

# Supplementary Materials

## Investigating the influence of data splitting on the predictive ability of QSAR/QSPR models

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## SUPPLEMENTARY MATERIALS REFERENCES

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- b Karelson M, Dobchev D, Tamm T, Tulp I, Jänes J, Tamm K, Lomaka A, Savchenko D & Karelson G (2008). Correlation of blood-brain penetration and human serum albumin binding with theoretical descriptors. *ARKIVOC* 16, 38-60.
- c Karelson M, Karelson G, Tamm T, Tulp I, Jänes J, Tamm K, Lomaka A, Savchenko D & Dobchev D (2009). QSAR study of pharmacological permeabilities. *ARKIVOC* 2, 218–238.
- d The JRC QMRF Q2-10-25-184 "QSAR for blood-brain barrier (BBB) partitioning" available at [http://qsar.db.jrc.ec.europa.eu/qmrf/search\\_catalogs.jsp?id=184&idstructure=](http://qsar.db.jrc.ec.europa.eu/qmrf/search_catalogs.jsp?id=184&idstructure=)
- e The JRC QMRF Q8-10-27-209 "QSAR for acute toxicity to algae" available at [http://qsar.db.jrc.ec.europa.eu/qmrf/search\\_catalogs.jsp?id=209&idstructure=](http://qsar.db.jrc.ec.europa.eu/qmrf/search_catalogs.jsp?id=209&idstructure=)
- f The JRC QMRF Q2-10-14-174 "QSAR for acute toxicity to fathead minnow" available at [http://qsar.db.jrc.ec.europa.eu/qmrf/search\\_catalogs.jsp?id=174&idstructure=](http://qsar.db.jrc.ec.europa.eu/qmrf/search_catalogs.jsp?id=174&idstructure=)
- g The JRC QMRF Q8-10-14-171 "QSAR for Relative Binding Affinity to Estrogen Receptor" available at [http://qsar.db.jrc.ec.europa.eu/qmrf/search\\_catalogs.jsp?id=171&idstructure=](http://qsar.db.jrc.ec.europa.eu/qmrf/search_catalogs.jsp?id=171&idstructure=)

CAS	Y (log(LC50) exp)	Average bond order (AM1)	Highest total interaction (AM1)	LPSA Low polarity (AM1)	part of SAS/
87-68-3	-3.46	1.180	-12.620	0.000	
67-72-1	-2.22	0.970	-11.720	0.000	
110-06-5	-2.11	0.970	-9.330	0.000	
110-54-3	-1.54	0.980	-12.170	0.000	
110-12-3	0.14	0.970	-11.970	0.000	
1634-04-4	0.88	0.970	-12.190	0.000	
75-05-8	1.60	0.000	0.000	0.000	
51-79-6	1.77	0.900	-12.170	0.000	
107-47-1	-0.70	0.970	-11.110	0.000	
106-47-8	-0.61	0.970	-12.130	0.000	
110-82-7	-1.27	0.970	-12.180	4.020	
102-69-2	-0.45	0.970	-12.030	4.020	
15045-43-9	0.12	0.970	-12.260	4.020	
732-26-3	-3.63	0.970	-12.250	4.200	
109-99-9	1.48	0.970	-12.170	5.360	
693-65-2	-1.70	0.970	-12.130	6.030	
91-65-6	-0.86	0.970	-11.980	6.030	
1198-55-6	-2.29	1.150	-12.620	8.400	
100-37-8	1.18	0.970	-12.030	11.170	
88-85-7	-2.65	1.060	-12.020	13.460	
107-41-5	1.96	0.970	-12.050	13.840	
281-23-2	-2.69	0.970	-12.170	14.740	
2921-88-2	-3.04	1.160	-12.630	15.400	
143-16-8	-2.38	0.970	-11.990	15.940	
100-41-4	-1.00	1.160	-12.900	16.080	
109-89-7	1.07	0.970	-11.990	16.220	
76-01-7	-1.43	0.970	-11.570	19.090	
77-74-7	0.82	0.970	-12.160	19.470	
75-65-0	1.94	0.970	-12.300	20.990	
115-20-8	0.30	0.960	-11.390	21.470	
499-83-2	0.28	0.960	-11.450	21.950	
67-63-0	2.16	0.970	-12.060	23.860	
600-36-2	0.15	0.970	-11.980	25.290	
109-60-4	-0.23	0.970	-11.690	25.760	
78-92-2	1.69	0.970	-12.060	25.960	
111-90-0	2.30	0.960	-12.120	26.720	
141-91-3	0.53	0.960	-12.060	26.720	
96-29-7	0.99	1.040	-12.160	27.490	
71-23-8	1.88	0.970	-12.140	27.670	
71-41-0	0.73	0.970	-12.140	27.670	
470-82-6	-0.18	0.970	-12.220	27.900	
123-15-9	-0.73	1.020	-11.980	28.090	
96-17-3	-0.94	1.030	-11.980	29.050	
67-56-1	2.96	0.970	-12.220	29.580	
64-17-5	2.50	0.970	-12.140	29.580	
143-08-8	-1.40	0.970	-12.140	29.970	
111-70-6	-0.53	0.970	-12.140	29.970	
128-37-0	-2.78	0.970	-12.170	30.150	
14548-46-0	-0.25	0.970	-11.960	30.160	

2176-62-7	-2.73	1.030	-12.720	30.210
111-27-3	-0.02	0.970	-12.140	30.920
71-36-3	1.37	0.970	-12.140	30.920
706-14-9	-0.98	0.970	-12.140	30.920
109-01-3	1.36	0.960	-12.060	32.850
97-02-9	-1.09	1.100	-12.110	36.260
6284-83-9	-3.09	1.130	-12.530	37.280
3698-83-7	-3.72	1.130	-12.270	37.730
58-90-2	-2.35	1.160	-12.480	37.790
2216-51-5	-0.92	0.970	-12.040	37.800
79-34-5	-0.92	0.960	-11.510	38.170
111-83-1	-2.36	0.970	-11.020	39.120
77-71-4	2.11	0.920	-12.310	39.120
2234-16-4	-1.21	0.970	-12.110	39.510
280-57-9	1.19	0.960	-12.260	40.930
109-65-9	-0.57	0.980	-11.020	41.030
629-04-9	-2.09	0.970	-11.020	41.030
6361-21-3	-1.68	0.970	-11.020	41.030
94-62-2	-1.56	1.080	-12.010	41.190
84-74-2	-2.44	1.010	-12.300	41.770
79-01-6	-0.47	1.160	-12.630	42.800
106-94-5	-0.26	0.980	-11.020	42.940
13952-84-6	0.58	0.970	-11.930	44.090
111-47-7	-0.74	0.980	-11.920	45.050
107-45-9	-0.72	0.970	-12.110	45.440
109-07-9	1.35	0.960	-12.060	45.540
75-97-8	-0.06	1.020	-12.230	45.800
693-16-3	-1.40	0.970	-12.010	46.000
14064-10-9	-2.31	1.000	-11.860	46.100
78-83-1	1.29	0.970	-12.070	46.760
105-53-3	-1.04	0.970	-12.100	47.140
768-94-5	-0.78	0.970	-12.150	48.120
118-79-6	-1.70	1.160	-12.310	48.410
563-80-4	1.00	1.030	-12.130	50.580
2016-57-1	-2.18	0.970	-12.010	50.680
88-06-2	-1.61	0.970	-11.910	51.050
529-19-1	-0.42	0.940	-12.070	51.150
66-76-2	-1.82	0.970	-12.010	51.150
100-64-1	0.26	1.020	-12.090	51.370
67-64-1	2.09	1.070	-12.270	51.530
109-85-3	0.84	0.960	-12.040	52.010
78-27-3	0.31	1.060	-12.180	52.280
4901-51-3	-2.75	1.160	-12.580	53.700
77-75-8	1.09	1.090	-12.180	53.830
2455-24-5	-0.69	1.040	-12.000	55.110
107-15-3	0.56	0.970	-12.010	55.260
111-86-4	-1.40	0.970	-12.010	55.730
761-65-9	-0.25	0.970	-12.010	55.730
108-10-1	0.72	0.970	-12.010	56.300
112-27-6	2.66	0.960	-12.120	56.300

110-58-7	0.31	0.970	-12.010	56.780
107-87-9	1.16	1.030	-12.130	57.730
111-46-6	2.85	0.960	-12.120	57.730
591-78-6	0.63	1.020	-12.130	57.930
75-09-2	0.59	0.970	-11.540	58.030
821-55-6	-0.97	1.000	-12.130	58.210
141-93-5	-1.51	1.000	-12.130	58.600
111-68-2	-0.72	0.970	-12.010	58.600
103-83-3	-0.55	1.010	-12.130	58.600
106-44-5	-0.82	1.030	-12.000	59.030
2370-63-0	-0.76	1.020	-12.000	59.030
110-43-0	0.06	1.010	-12.130	59.160
19549-98-5	-0.46	1.050	-12.070	59.960
90-59-5	-2.52	1.190	-11.990	61.330
387-45-1	-1.23	1.110	-12.150	61.520
502-56-7	-0.66	0.970	-12.070	61.950
1482-15-1	0.26	1.070	-12.060	62.410
1891-95-8	-0.89	1.280	-12.450	62.540
544-40-1	-1.61	1.080	-12.450	62.540
590-86-3	-1.42	1.050	-12.030	63.140
613-45-6	1.22	0.970	-12.010	63.170
112-05-0	-0.18	0.970	-12.080	63.660
104-76-7	-0.66	1.000	-12.130	63.750
98-54-4	-1.46	1.060	-12.180	64.090
115-19-5	1.59	1.110	-12.310	64.760
2869-34-3	-3.48	0.970	-12.010	65.310
140-31-8	1.23	0.960	-12.060	65.370
79-00-5	-0.21	0.970	-11.310	65.560
121-14-2	-0.87	1.090	-12.010	65.970
3428-24-8	-2.30	1.140	-12.550	66.160
100-79-8	2.10	0.960	-12.120	66.800
1126-79-0	-1.42	1.030	-11.990	67.890
142-62-1	0.44	0.970	-12.140	68.230
107-19-7	-1.58	1.050	-12.020	68.550
100-25-4	-2.37	0.980	-12.440	68.710
80-52-4	-0.42	0.970	-12.080	69.660
78-93-3	1.65	1.040	-12.130	69.660
616-86-4	-0.85	1.030	-12.150	70.230
71-55-6	-0.45	0.970	-11.460	71.570
629-19-6	-1.76	0.970	-9.210	72.050
552-89-6	-1.02	0.970	-12.170	73.510
928-96-1	0.58	1.020	-12.040	73.700
109-75-1	0.43	1.020	-12.040	73.700
464-45-9	-0.39	0.970	-12.120	74.500
58-08-2	-0.11	0.960	-12.190	74.930
100-10-7	-0.51	1.120	-12.010	75.260
271-89-6	-0.93	1.120	-12.320	76.530
1745-81-9	-0.95	1.000	-12.220	76.680
2437-25-4	-2.62	1.030	-12.030	76.810
78-96-6	1.53	0.960	-12.050	77.010

534-52-1	-2.06	1.090	-12.170	77.060
116-06-3	-2.34	0.970	-11.090	77.340
107-12-0	1.44	1.210	-12.030	78.120
16879-02-0	0.22	1.090	-12.390	79.200
70-30-4	-4.29	1.140	-11.980	79.330
95-01-2	-1.02	1.170	-12.000	79.460
2973-76-4	-0.59	1.140	-12.010	79.520
96-13-9	-0.49	0.960	-10.900	79.680
102-71-6	1.90	0.960	-12.050	81.110
593-08-8	-2.74	1.000	-12.080	81.210
5922-60-1	-0.73	1.260	-12.450	81.430
141-78-6	0.42	0.970	-12.170	82.070
107-14-2	-1.75	1.350	-11.290	82.390
1689-83-4	-1.74	1.060	-12.360	82.900
105-14-6	0.33	1.000	-12.030	82.930
1740-19-8	-2.16	0.970	-11.960	83.030
142-92-7	-1.52	0.970	-12.170	83.410
95-47-6	-0.81	0.970	-12.170	83.410
96-22-0	1.25	1.030	-12.130	83.970
107-10-8	0.72	1.020	-12.070	84.930
2495-37-6	-1.58	1.230	-11.910	85.320
683-72-7	0.28	1.010	-12.490	85.930
121-32-4	-0.28	1.120	-12.010	86.080
330-54-1	-1.22	1.000	-12.160	87.990
110-88-3	1.82	0.950	-12.010	88.750
105-75-9	-2.56	1.000	-12.150	88.810
80-46-6	-1.80	0.970	-12.160	88.810
110-73-6	1.22	0.970	-12.190	88.830
2460-49-3	-1.64	1.110	-12.190	89.070
102-27-2	-0.44	1.000	-12.130	89.440
927-74-2	-0.29	1.150	-12.010	89.700
78-51-3	-1.55	0.960	-12.050	90.000
120-83-2	-1.32	0.960	-12.420	90.590
100-01-6	-0.04	1.120	-12.370	91.800
108-94-1	0.80	1.020	-12.100	91.810
764-13-6	-1.46	0.970	-12.290	93.070
999-61-1	-1.59	1.010	-12.070	94.170
24544-04-5	-1.06	0.990	-12.000	94.540
112-12-9	-2.06	1.000	-12.070	94.860
105-67-9	-0.87	0.970	-12.170	94.970
7212-44-4	-2.19	1.000	-12.070	95.720
94-09-7	-0.67	1.070	-12.160	96.060
573-56-8	-0.67	1.110	-12.260	96.150
109-64-8	-1.98	0.970	-12.130	96.700
111-25-1	-1.68	1.110	-11.990	96.700
120-21-8	-0.87	1.100	-12.150	97.270
17584-12-2	0.88	1.060	-12.180	97.310
59-50-7	-1.42	0.960	-12.190	98.190
13071-79-9	-4.34	0.910	-8.700	98.290
622-40-2	1.32	0.960	-12.060	99.250

110-65-6	-0.21	1.130	-11.910	99.690
118-61-6	-0.92	0.970	-12.420	100.200
78-90-0	1.13	0.970	-12.030	101.340
872-31-1	-1.42	1.070	-12.620	101.970
109-73-9	0.56	0.970	-12.050	104.010
75-07-0	-0.12	1.120	-12.010	104.440
141-03-7	-1.71	0.970	-12.080	104.590
79-20-9	0.68	0.970	-12.210	104.970
111-42-2	1.65	0.960	-12.050	105.350
106-42-3	-1.08	1.100	-12.180	105.970
99-08-1	-0.73	1.130	-12.010	106.310
109-77-3	-2.07	1.610	-11.820	106.630
10031-82-0	-0.73	0.970	-12.170	106.840
615-65-6	-0.60	1.090	-12.000	106.970
122-03-2	-1.35	1.000	-12.010	107.130
497-37-0	0.31	0.970	-12.140	107.500
1072-97-5	0.01	1.020	-12.330	107.690
123-07-9	-1.07	0.970	-12.140	109.740
109-76-2	1.21	0.970	-12.010	109.740
619-50-1	-0.88	0.970	-12.220	111.080
127-00-4	0.41	0.970	-11.060	111.080
141-43-5	1.53	0.960	-12.050	111.270
645-56-7	-1.09	0.970	-12.140	111.400
126-81-8	1.91	1.050	-12.020	111.650
555-16-8	-1.18	1.010	-12.060	111.820
2416-94-6	-1.22	0.960	-12.170	112.480
83-34-1	-1.17	0.970	-12.220	112.540
709-98-8	-1.40	1.030	-12.110	112.740
3126-90-7	-2.49	0.970	-12.150	113.370
100-02-7	-0.49	1.070	-12.380	114.260
17754-90-4	-1.56	0.970	-12.200	115.180
87-86-5	-3.04	0.970	-12.030	115.440
540-88-5	0.45	0.970	-12.260	115.470
91-20-3	-1.32	0.960	-12.420	115.530
1761-61-1	-2.19	1.120	-12.000	115.790
625-86-5	-0.13	1.030	-12.180	117.340
1689-84-5	-1.34	1.280	-12.340	117.670
67-66-3	-0.23	0.970	-12.150	117.760
329-71-5	-1.74	0.970	-12.160	118.030
874-42-0	-1.99	1.010	-12.000	118.400
2032-59-9	-2.03	0.940	-12.110	118.460
2499-95-8	-2.15	1.000	-12.160	118.750
81-19-6	-2.37	0.960	-11.350	118.970
105-99-7	-1.85	0.970	-12.070	119.100
120-82-1	-1.78	0.970	-12.520	119.100
4798-44-1	-0.52	1.020	-12.030	119.190
2008-58-4	0.39	0.960	-12.540	120.110
121-33-5	-0.26	1.140	-12.010	120.370
95-57-8	-1.05	0.970	-12.090	120.540
4655-34-9	-0.53	1.010	-12.060	123.410



108-90-7	-0.82	0.970	-12.170	123.510
527-60-6	-1.02	1.010	-11.930	125.930
91-88-3	-0.53	0.960	-12.070	125.960
84-66-2	-0.84	0.970	-12.160	126.660
121-69-7	-0.28	1.000	-12.130	127.360
111-15-9	-0.50	0.970	-12.060	127.870
104-88-1	-1.81	1.010	-12.010	128.890
22104-62-7	-1.18	1.010	-12.010	129.150
79-95-8	-2.44	0.970	-12.140	129.180
13608-87-2	-2.05	1.010	-12.260	129.620
822-86-6	-0.92	1.030	-12.170	129.780
2150-47-2	-0.56	1.080	-12.210	129.780
95-63-6	-1.19	0.970	-12.160	131.060
110-40-7	-1.98	0.970	-11.030	131.120
693-54-9	-1.51	0.970	-12.110	131.120
91-66-7	-0.96	0.960	-12.070	135.890
939-23-1	-0.98	0.970	-12.090	136.000
51-28-5	-1.23	1.070	-11.980	136.020
3066-71-5	-2.02	1.000	-12.070	136.040
350-46-9	-0.70	1.080	-12.390	136.270
629-40-3	0.59	1.150	-12.030	136.470
298-04-4	-2.00	0.950	-10.580	137.520
1962-75-0	-2.67	0.970	-12.080	137.580
65-45-2	-0.13	1.050	-12.490	138.590
90-02-8	-1.73	1.120	-12.000	139.770
88-75-5	0.06	1.070	-12.390	140.150
111-69-3	1.25	1.220	-12.030	140.220
134-62-3	-0.24	0.970	-12.080	140.650
496-16-2	-0.17	1.050	-12.030	140.650
104-90-5	-0.17	1.010	-12.140	140.990
99-97-8	-0.44	0.970	-12.030	141.200
106-63-8	-1.79	1.010	-12.070	141.470
4460-86-0	-0.60	1.010	-12.170	141.830
619-50-1	-0.88	1.040	-12.150	142.150
141-28-6	-1.05	0.960	-12.360	143.590
5372-81-6	-1.37	1.020	-12.210	144.160
498-66-8	-0.97	1.020	-12.280	145.520
6175-49-1	-2.19	1.040	-12.010	146.230
945-51-7	-0.36	1.010	-12.000	146.410
123-86-4	-0.81	1.080	-12.010	146.620
15128-82-2	0.08	1.080	-12.490	147.540
91-22-5	-0.22	1.110	-12.200	147.660
67-68-5	2.64	0.820	-12.620	148.860
66-25-1	-0.76	1.000	-12.090	148.880
1563-66-2	-2.42	0.990	-12.170	149.390
88-68-6	0.46	1.040	-12.490	151.730
868-77-9	0.24	1.010	-12.120	152.800
1204-21-3	-3.59	1.030	-11.250	152.910
314-40-9	-0.15	0.960	-11.890	153.310
98-95-3	-0.01	0.970	-12.450	153.700

107-07-3	-0.18	0.960	-11.040	153.790
1126-46-1	-1.19	0.970	-12.210	155.010
57-43-2	-0.42	1.070	-12.200	155.830
148-53-8	-1.80	1.090	-11.990	155.990
541-73-1	-1.26	0.970	-12.470	157.010
95-76-1	-1.33	1.150	-12.500	157.070
18368-63-3	0.26	1.020	-12.210	159.100
2243-27-8	-1.42	0.970	-12.150	159.490
513-81-5	-1.08	0.960	-12.590	164.070
928-97-2	0.43	1.290	-11.900	164.170
621-08-9	-0.46	0.960	-12.550	164.260
13209-15-9	-2.98	0.960	-11.190	164.390
108-99-6	0.19	1.020	-12.160	164.400
95-50-1	-1.19	0.970	-12.560	165.030
123-66-0	-1.21	1.010	-12.260	166.230
104-13-2	-1.17	0.970	-12.140	168.280
96-18-4	-0.41	0.960	-11.080	168.460
95-51-2	-1.35	1.010	-12.300	168.910
100-70-9	0.84	1.160	-12.460	170.650
1129-35-7	-0.54	1.050	-12.220	171.070
120-80-9	-1.08	0.970	-12.160	171.630
100-52-7	-1.03	1.020	-12.010	171.710
108-89-4	0.64	1.020	-12.160	172.860
589-16-2	-0.22	0.970	-12.140	173.330
119-34-6	-0.63	1.050	-12.480	173.460
693-98-1	0.54	1.040	-12.210	173.730
500-22-1	-0.81	0.970	-12.180	174.620
106-40-1	-0.56	1.080	-12.260	174.820
123-72-8	-0.69	1.000	-12.080	176.400
100-71-0	0.59	1.010	-12.100	176.810
55-21-0	0.74	0.960	-12.500	178.010
818-61-1	-1.38	0.940	-12.090	178.070
75-89-8	0.08	0.950	-12.140	178.400
88-30-2	-1.36	1.050	-12.350	178.690
538-68-1	-1.94	0.970	-12.140	178.710
583-53-9	-1.77	0.970	-12.320	179.410
150-76-5	-0.05	1.010	-12.200	179.470
122-99-6	0.40	0.960	-12.110	180.360
123-54-6	0.13	1.090	-12.180	185.130
97-23-4	-2.94	0.960	-12.060	186.560
542-75-6	-2.67	1.080	-11.040	188.380
115-32-2	-2.79	0.960	-11.390	188.850
142-96-1	-0.61	0.960	-12.390	188.950
106-49-0	0.17	0.960	-12.160	190.150
13909-73-4	-0.02	1.080	-12.160	192.090
110-00-9	-0.05	1.060	-12.680	192.150
98-82-8	-1.28	0.970	-12.050	192.890
2905-69-3	-1.17	1.090	-12.170	193.000
110-93-0	-0.17	0.960	-12.200	194.610
1746-23-2	-2.51	1.000	-12.290	196.110

100-61-8	-0.03	0.960	-12.130	196.950
78-87-5	0.05	0.970	-10.860	197.030
115-90-2	-0.85	0.900	-12.100	197.370
120-07-0	0.61	0.960	-12.050	197.600
150-78-7	-0.07	1.000	-12.200	198.110
621-42-1	0.87	1.080	-12.290	198.110
109-06-8	0.98	1.020	-12.210	201.210
39905-57-2	-1.81	0.990	-12.150	202.280
127-18-4	-1.00	0.970	-12.150	202.380
50-06-6	0.32	0.940	-12.180	202.980
111-13-7	-0.55	0.970	-12.010	204.100
932-16-1	0.10	1.030	-12.490	207.300
96-05-9	-2.11	1.070	-11.960	207.840
628-76-2	-0.75	1.000	-12.260	209.050
103-90-2	0.73	1.000	-12.260	209.430
2759-28-6	-0.57	0.960	-12.010	209.620
2859-67-8	0.04	1.000	-12.130	212.270
14321-27-8	-0.37	0.970	-11.990	213.190
614-80-2	-0.75	0.970	-12.170	214.590
95-75-0	-1.74	1.280	-11.870	215.800
110-62-3	-0.82	0.970	-12.400	216.560
29553-26-2	0.56	0.960	-11.880	216.900
108-88-3	-0.43	0.970	-12.160	219.160
454-89-7	-2.28	1.000	-12.010	219.680
127-66-2	-0.11	1.040	-12.320	220.060
607-81-8	-1.66	0.970	-11.910	221.840
103-05-9	-0.39	0.970	-12.110	223.750
62-53-3	0.05	0.960	-12.540	227.880
1122-54-9	0.14	1.060	-12.260	229.630
110-86-1	0.10	1.060	-12.170	230.090
121-73-3	-0.92	0.970	-10.860	231.870
90-15-3	-1.49	1.080	-12.520	236.090
107-06-2	0.14	0.970	-11.120	237.310
368-77-4	-0.55	1.060	-12.450	239.070
464-48-2	-0.95	1.010	-12.040	239.960
95-52-3	-0.75	0.970	-11.040	240.730
98-86-2	0.13	1.010	-12.260	242.900
133-11-9	-1.68	1.040	-12.360	243.720
393-39-5	-0.78	1.050	-12.460	246.190
100-46-9	-0.02	0.970	-12.110	251.490
5292-45-5	-1.56	1.040	-12.080	251.920
93-91-4	-2.17	1.030	-12.210	253.610
121-87-9	-0.93	1.120	-12.550	258.720
14548-45-9	-1.11	1.020	-12.220	259.680
2104-64-5	-3.61	0.980	-12.060	262.620
99-03-6	0.45	1.040	-12.220	268.250
142-28-9	-0.01	0.970	-11.060	268.480
150-19-6	-0.22	1.140	-12.440	269.370
71-43-2	-0.65	0.970	-12.590	272.290
75-47-8	-2.13	0.960	-12.080	272.700

63-25-2	-1.36	1.020	-12.170	287.300
1871-57-4	-2.82	1.050	-10.960	289.260
87-17-2	-1.73	1.010	-12.470	292.460
67-36-7	-1.63	1.020	-12.010	298.320
79-77-6	-1.58	1.000	-11.960	301.400
110-56-5	-0.39	0.970	-11.030	301.660
609-23-4	-2.59	1.080	-11.860	303.400
111-26-2	-0.25	1.020	-12.490	307.070
90-43-7	-1.44	0.960	-12.520	322.390
106-48-9	-1.32	1.090	-12.570	325.220
111-87-5	-0.98	1.000	-12.490	328.140
132-64-9	-2.05	1.030	-12.540	330.650
608-71-9	-3.72	1.160	-12.400	332.500
119-61-9	-1.09	0.990	-12.500	335.880
118-55-8	-2.26	1.020	-12.420	340.870
831-82-3	-1.58	0.960	-12.540	342.870
1484-26-0	-1.34	1.040	-12.030	352.510
623-25-6	-3.65	0.960	-10.960	353.260
52645-53-1	-4.39	0.980	-11.960	374.120
10453-86-8	-4.74	1.000	-11.910	375.950
3923-52-2	-1.27	1.020	-12.510	386.810
108-95-2	-0.46	0.920	-12.460	408.500
84-62-8	-3.60	0.960	-12.510	514.740
115-86-6	-2.57	0.950	-12.570	548.680
60-29-7	1.54	0.970	-12.130	0.000
771-60-8	-0.69	1.140	-13.990	8.400
471-77-2	-2.31	0.970	-11.480	16.220
108-93-0	0.85	0.970	-12.070	25.780
126-73-8	-1.45	0.950	-12.090	35.030
112-20-9	-1.82	0.970	-12.140	38.000
107-29-9	0.11	1.090	-12.210	42.800
124-22-1	-3.26	0.970	-12.010	60.710
103-76-4	1.69	0.960	-12.050	66.990
514-10-3	-2.10	1.000	-11.920	76.120
96-80-0	0.14	1.010	-12.070	83.500
619-80-7	-0.10	0.970	-12.450	92.410
104-40-5	-3.20	0.970	-12.130	99.770
23135-22-0	-1.51	0.940	-12.180	106.880
5835-26-7	-2.54	1.000	-11.890	107.960
123-91-1	2.07	0.960	-12.160	116.420
635-93-8	-2.31	1.120	-12.000	125.140
95-48-7	-0.89	0.970	-12.190	134.320
333-41-5	-1.51	0.990	-12.030	140.800
16752-77-5	-1.89	0.970	-12.170	151.180
121-75-5	-1.37	0.950	-10.600	159.750
16245-79-7	-3.23	0.970	-12.140	167.190
70-69-9	-0.01	1.120	-12.110	174.660
1647-16-1	-2.68	1.040	-12.050	183.280
15972-60-8	-1.73	0.960	-11.210	192.120
114-26-1	-1.38	1.020	-12.120	199.580

109-97-7	0.50	1.050	-12.790	210.240
786-19-6	-3.15	0.900	-9.160	214.770
1080-32-6	0.17	0.940	-12.080	222.350
58-27-5	-3.19	1.070	-12.180	232.870
920-66-1	0.16	0.940	-12.040	239.390
83-32-9	-1.95	1.060	-12.170	249.400
371-40-4	-0.82	0.960	-12.570	265.970
86-50-0	-3.70	0.970	-10.460	276.130
529-20-4	-0.36	0.960	-12.420	279.860
1689-82-3	-2.23	1.080	-12.450	288.800
620-88-2	-1.91	1.020	-12.390	297.880
525-82-6	-1.80	1.070	-12.440	330.010
83-79-4	-4.88	1.090	-11.900	338.110
112-30-1	-1.82	1.080	-12.020	349.880
122-39-4	-1.65	0.960	-12.550	367.240
882-33-7	-3.30	0.960	-8.670	375.870
791-28-6	-0.71	0.940	-12.380	392.650
101-84-8	-1.63	0.960	-12.560	414.460
51630-58-1	-4.92	0.990	-11.730	455.530
70124-77-5	-6.38	0.990	-11.710	532.050

Count of H-acceptor sites (AM1) (all LogP	Z to 1	(kX)	(Y/kX)	(kY/kX)	Duplex
6	4.780	1	1	1	1
6	4.140	1	1	1	1
2	4.220	1	1	1	1
0	3.870	1	1	1	1
2	0.860	1	1	1	1
1	0.940	1	1	1	1
0	-0.340	1	1	1	1
3	-0.150	1	1	1	1
1	3.320	1	1	2	1
1	3.210	1	1	2	1
0	3.440	1	1	1	1
1	2.790	1	1	2	1
1	2.400	1	2	2	1
1	7.400	1	1	1	1
1	0.460	1	1	1	1
1	4.040	1	1	1	1
1	2.970	1	1	1	1
6	4.290	1	1	1	1
2	0.320	1	1	1	1
5	3.690	1	1	1	1
2	-0.670	1	1	1	1
0	3.980	1	1	1	1
6	5.120	1	1	1	1
1	4.770	1	1	1	1
4	3.400	1	1	1	1
1	0.580	1	1	1	1
5	3.630	1	1	1	1
1	1.530	1	1	1	1
1	0.350	1	1	1	1
4	1.420	1	1	2	1
4	0.090	1	1	1	1
1	0.050	1	1	1	1
1	1.930	1	1	2	1
3	1.950	1	1	1	1
1	0.610	1	1	1	1
3	-0.540	1	1	1	1
2	0.320	1	2	2	1
2	0.650	1	1	2	1
1	0.250	1	1	1	1
1	1.560	2	1	1	1
1	2.760	1	1	1	1
1	1.670	1	2	1	1
1	1.140	1	1	2	1
1	-0.770	1	1	1	1
1	-0.310	1	2	2	1
1	4.260	1	1	1	1
1	2.720	1	1	2	1
1	6.070	1	1	1	1
2	2.140	1	1	1	1

6	4.340	1	1	1	1	1
1	2.030	1	1	1	1	1
1	0.880	2	1	1	1	1
1	2.970	1	2	1	1	1
2	-0.100	1	1	1	1	1
5	1.840	1	1	1	1	1
7	2.650	1	1	1	1	1
6	2.490	1	1	1	1	1
5	4.450	1	1	1	1	1
1	3.230	2	1	1	1	1
4	2.390	1	1	1	1	1
1	4.890	1	1	1	1	1
4	-0.650	1	1	1	1	1
2	2.790	1	1	1	1	1
2	0.690	1	1	1	1	1
1	2.750	1	1	1	1	1
1	4.360	1	2	2	1	1
1	3.800	1	1	1	2	1
3	3.340	1	1	1	1	1
6	6.440	1	1	1	1	1
3	2.420	1	1	1	1	1
1	2.100	1	1	1	1	1
1	0.700	1	1	1	1	1
1	2.960	1	1	1	1	1
1	2.430	1	2	2	2	1
2	-0.440	1	1	1	1	1
1	0.970	1	1	1	1	1
1	2.820	1	2	1	1	1
2	6.240	1	1	1	1	1
1	0.760	1	1	1	1	1
4	1.070	1	1	1	1	1
1	2.440	1	1	1	1	1
4	4.020	1	1	1	1	1
1	0.560	1	1	1	1	1
1	4.100	1	1	1	2	1
1	4.020	1	2	1	2	1
5	2.070	1	1	1	1	1
1	3.570	1	2	2	1	1
2	1.200	1	1	1	1	1
1	-0.240	2	1	1	1	1
2	-0.670	1	1	1	1	1
1	1.730	2	1	1	1	1
5	4.210	1	1	1	1	1
1	0.860	1	1	1	1	1
1	0.880	1	2	1	1	1
1	0.970	1	1	2	2	1
1	3.040	1	1	1	1	1
1	2.060	1	2	1	1	1
1	0.480	1	1	1	1	1
4	-1.240	1	1	1	1	1

1	1.490	1	1	1	1	1
1	0.910	1	1	1	1	1
3	-1.300	1	1	1	1	1
1	1.380	1	2	2	2	1
2	1.250	1	1	1	1	1
1	3.140	2	1	1	2	1
1	3.730	1	2	1	1	1
1	2.570	1	2	2	2	1
1	2.370	1	2	2	2	1
1	1.360	1	1	1	1	1
1	1.780	1	2	2	2	1
1	1.980	1	2	2	1	1
1	2.320	2	1	1	1	1
4	3.830	1	1	1	1	1
5	1.540	1	1	1	1	1
1	2.810	1	1	1	1	1
1	1.260	1	1	1	1	1
4	2.690	1	1	1	1	1
4	3.690	1	1	2	1	1
1	3.120	1	2	1	1	1
2	-0.460	1	1	1	1	1
2	3.470	1	1	1	1	1
1	2.910	1	1	2	1	1
0	3.760	1	1	1	1	1
1	0.280	1	1	1	1	1
1	5.680	1	1	1	1	1
3	-0.680	1	1	1	1	1
3	2.050	2	1	1	1	1
2	2.940	1	1	1	1	1
4	2.900	2	1	1	1	1
3	-0.070	1	2	2	2	1
1	1.230	1	1	1	1	1
2	1.920	1	1	1	1	1
1	3.960	1	1	1	1	1
4	1.460	1	1	1	1	1
2	1.230	1	1	1	1	1
1	0.290	1	1	1	1	1
4	2.470	1	1	1	1	1
3	2.490	1	1	1	1	1
2	3.860	1	1	1	1	1
1	3.420	1	1	1	1	1
1	1.340	2	2	1	1	1
1	1.340	1	1	2	2	1
1	2.580	1	1	1	1	1
6	-0.070	1	1	1	1	1
2	1.810	1	1	1	1	1
4	2.170	1	1	1	1	1
1	2.100	1	1	1	1	1
1	4.900	2	1	1	1	1
2	-0.960	1	1	1	1	1



5	2.560	1	1	1	2	1
5	1.120	1	1	1	1	1
1	0.160	1	1	1	1	1
3	1.780	2	1	1	1	1
8	7.540	1	1	1	1	1
3	1.710	1	2	1	1	1
4	2.090	2	1	2	1	1
3	0.630	1	1	1	1	1
4	-1.750	1	1	1	1	1
1	5.020	1	1	1	1	1
3	1.910	2	1	1	1	1
2	0.730	1	1	1	1	1
2	0.450	1	1	1	1	1
5	1.750	1	1	1	1	1
2	0.350	1	2	2	2	1
2	6.500	1	1	1	1	1
2	2.790	1	1	1	1	1
2	1.730	1	1	1	1	1
1	0.790	1	1	1	1	1
1	1.310	1	1	1	1	1
1	-0.370	1	1	1	1	1
5	0.900	1	1	1	1	1
3	1.880	1	1	1	1	1
1	3.420	1	1	2	1	1
3	-0.430	1	1	1	1	1
4	3.910	1	1	1	1	1
1	3.980	2	1	1	1	1
2	1.910	1	1	1	1	1
4	3.260	1	2	1	1	1
1	2.810	1	1	1	1	1
1	-0.500	1	1	1	1	1
7	4.090	1	1	1	1	1
3	3.060	1	1	1	1	1
3	1.310	1	1	1	2	1
1	0.810	1	1	1	1	1
1	3.310	1	1	1	1	1
3	0.350	1	1	1	1	1
1	3.180	1	2	2	2	1
1	4.090	2	1	2	1	1
1	2.300	1	1	1	1	1
1	4.490	1	2	1	1	1
3	1.860	1	1	1	1	1
5	1.910	2	1	1	1	1
4	3.820	1	1	1	1	1
4	2.280	1	2	1	1	1
4	2.000	1	1	2	1	1
4	-0.210	2	1	1	1	1
2	3.100	2	1	1	1	1
5	4.480	1	1	1	1	1
3	-0.450	1	1	1	1	1

2	-1.830	1	1	1	1	1
3	2.410	1	1	1	1	1
2	-0.910	1	1	1	1	1
2	2.620	1	1	1	1	1
2	-1.220	1	1	1	1	1
1	-0.220	1	1	1	1	1
4	3.540	1	1	1	1	1
2	0.180	1	1	1	1	1
3	-1.430	1	1	1	1	1
0	2.700	1	1	1	1	1
2	2.310	1	1	1	1	1
2	-0.500	1	1	1	1	1
2	2.450	1	2	2	2	1
4	1.380	1	1	1	1	1
1	3.070	1	1	1	1	1
1	1.020	1	1	1	1	1
3	1.390	1	1	1	1	1
1	2.580	1	1	1	1	1
2	-1.490	2	1	1	1	1
4	2.020	1	1	1	1	1
2	0.140	1	1	1	1	1
2	-1.310	1	1	1	1	1
1	3.200	2	1	1	1	1
2	0.510	1	1	1	1	1
2	0.220	1	2	1	1	1
5	2.800	1	1	2	2	1
4	3.370	1	1	2	1	1
4	3.070	1	2	1	1	1
4	5.530	1	1	1	1	1
3	1.910	1	1	1	1	1
6	1.920	1	1	1	1	1
8	4.960	1	1	1	1	1
2	1.380	2	1	1	1	1
2	2.480	1	1	1	1	1
3	3.150	1	1	1	1	1
1	2.620	2	1	1	1	1
4	2.990	1	1	1	1	1
2	1.200	1	1	1	1	1
2	4.220	1	1	1	1	1
3	3.110	1	1	1	2	1
4	2.160	1	1	1	1	1
2	3.390	1	1	2	2	1
4	4.640	1	1	1	1	1
4	3.820	1	1	2	1	1
3	4.020	1	1	1	2	1
1	1.120	1	1	1	1	1
4	1.250	1	1	1	1	1
3	1.210	2	1	1	1	1
4	1.710	1	2	1	1	1
2	2.250	2	1	2	1	1

1	1.940	1	1	1	1	1
3	1.740	1	1	1	1	1
2	2.490	1	1	1	2	1
4	2.470	1	1	1	1	1
1	2.310	1	1	1	1	1
3	0.650	1	1	1	1	1
2	2.100	1	1	1	1	1
3	1.500	1	1	1	1	1
4	4.720	1	1	1	1	1
4	3.570	1	1	1	1	1
3	3.140	1	1	1	1	1
4	2.220	1	1	1	1	1
0	3.780	2	2	1	1	1
2	1.990	1	1	1	1	1
0	4.500	1	1	1	1	1
1	3.310	1	1	1	1	1
2	2.720	1	2	1	2	1
3	2.540	1	1	1	1	1
2	2.780	1	1	1	1	1
3	1.800	1	2	1	1	1
2	0.590	1	1	1	1	1
5	4.020	1	1	1	1	1
4	5.530	1	1	1	1	1
3	1.280	1	1	1	1	1
2	1.810	1	1	1	1	1
3	1.850	1	1	1	1	1
2	-0.320	1	1	1	1	1
2	2.310	1	1	1	2	1
1	1.700	1	1	1	2	1
1	2.490	1	2	2	1	1
1	2.820	1	1	1	2	1
2	2.220	1	2	1	1	1
2	2.580	1	1	2	2	1
2	2.800	1	2	1	1	1
2	2.150	1	1	1	1	1
5	2.450	1	1	1	1	1
0	2.560	1	1	1	1	1
1	4.400	1	1	1	1	1
1	2.260	1	1	1	1	1
2	0.510	1	1	1	1	1
4	1.010	1	1	1	1	1
2	1.580	1	1	1	1	1
1	-1.350	1	1	1	1	1
3	1.400	1	1	1	1	1
4	2.320	2	1	1	1	1
3	0.350	1	1	1	2	1
3	0.470	1	1	2	1	1
4	2.390	1	1	1	1	1
5	2.110	1	1	1	1	1
2	1.850	1	1	1	1	1

2	0.030	1	1	1	1	1
3	2.900	1	1	1	2	1
1	2.210	1	1	1	1	1
3	1.370	1	1	1	2	1
2	3.600	1	1	1	1	1
3	2.690	1	1	1	2	1
2	2.090	1	1	1	1	1
1	3.650	1	1	1	1	1
2	0.880	1	1	1	1	1
1	0.120	1	1	1	1	1
1	1.460	1	1	1	1	1
4	5.170	1	1	1	1	1
1	1.310	1	2	2	2	1
2	3.380	1	1	2	1	1
3	2.840	1	1	1	1	1
1	3.150	1	1	1	2	1
3	1.980	1	1	1	1	1
2	1.900	1	1	1	1	1
2	0.500	1	1	1	1	1
3	1.720	1	1	1	1	1
0	3.150	1	1	1	1	1
1	1.480	2	1	1	1	1
1	1.220	1	1	1	1	1
1	1.960	1	2	1	1	1
4	0.960	1	1	1	1	1
2	0.600	1	1	1	1	1
0	3.120	1	1	1	1	1
2	2.260	1	1	2	1	1
3	1.300	1	1	1	1	1
1	1.690	1	1	1	1	1
2	0.640	1	1	1	1	1
4	1.450	1	1	1	1	1
4	0.410	1	1	1	1	1
6	3.000	1	1	1	1	1
0	4.910	2	1	1	1	1
2	3.640	1	1	1	1	1
2	1.340	1	2	2	2	1
2	1.160	1	1	1	1	1
2	-0.540	2	1	1	1	1
4	4.260	1	1	1	1	1
2	1.600	1	1	1	1	1
6	6.060	2	1	1	1	1
2	1.830	1	1	1	1	1
1	1.390	1	1	1	1	1
4	1.120	1	1	1	1	1
1	1.340	1	1	1	1	1
0	3.660	2	1	1	1	1
1	2.790	1	1	1	2	1
1	2.140	1	1	1	1	1
0	4.840	1	1	1	1	1

1	1.660	2	1	1	1	1
2	1.990	1	1	1	1	1
5	2.230	2	1	1	1	1
3	0.440	1	1	2	2	1
2	2.150	1	1	1	1	1
3	0.730	1	2	1	1	1
1	1.110	1	1	1	1	1
2	3.660	1	1	1	1	1
0	3.150	1	1	1	1	1
5	1.470	1	1	1	1	1
1	1.950	1	1	1	1	1
1	0.650	1	1	1	1	1
2	1.570	1	1	1	1	1
3	0.720	1	1	1	1	1
3	0.320	1	2	1	1	1
2	1.760	1	1	1	1	1
2	0.600	1	1	1	1	1
1	2.040	1	1	1	1	1
1	2.930	1	1	1	1	1
4	3.510	1	1	1	1	1
1	2.860	1	1	1	1	1
5	1.030	1	1	1	1	1
0	2.730	1	1	1	1	1
4	2.470	1	1	1	1	1
1	1.680	1	1	1	1	1
4	2.760	1	1	1	1	1
1	2.570	2	1	1	1	1
1	0.900	2	1	1	1	1
2	0.480	1	2	1	2	1
2	1.020	1	1	1	1	1
2	3.180	1	1	1	1	1
1	2.840	1	1	1	1	1
2	1.480	1	1	2	1	1
4	2.460	1	1	1	1	1
1	2.640	1	1	1	1	1
2	2.760	1	1	1	1	1
1	1.580	1	1	1	1	1
4	3.150	1	1	1	1	1
5	2.620	2	1	1	1	1
1	1.090	1	1	1	1	1
4	2.700	1	1	1	1	1
2	1.050	2	1	1	1	1
1	2.670	1	1	1	1	1
3	2.970	1	1	1	1	1
5	3.850	1	1	1	1	1
2	0.900	1	1	1	1	1
2	2.000	1	1	1	1	1
1	2.050	1	1	1	1	1
0	2.130	1	1	1	1	1
3	3.540	1	1	1	1	1

3	2.360	2	1	1	1	1
2	1.560	1	1	1	1	1
3	3.270	2	1	1	1	1
2	3.960	1	1	1	2	1
2	2.820	1	1	1	1	1
2	2.240	1	1	1	1	1
4	4.800	1	1	1	1	1
2	1.980	1	1	1	2	1
1	3.360	1	1	1	1	1
0	3.300	1	1	1	1	1
1	2.590	1	1	2	1	1
1	4.120	1	1	1	1	1
6	4.690	1	1	1	1	1
1	3.180	1	1	1	1	1
3	4.120	1	1	1	1	1
2	3.750	2	1	1	1	1
2	2.790	1	1	1	1	1
2	3.270	1	1	1	1	1
5	6.500	1	1	1	1	1
3	6.180	1	1	1	1	1
1	2.710	1	1	1	1	1
1	1.960	1	1	1	1	1
4	4.530	1	1	1	1	1
4	4.590	1	1	1	1	1
1	0.890	1	2	2	1	2
6	2.220	1	1	1	1	2
5	2.590	1	1	1	1	2
1	1.230	1	2	1	1	2
4	3.530	1	1	1	1	2
1	4.570	1	1	1	1	2
2	-0.140	1	1	1	1	2
1	5.160	1	1	1	1	2
3	-0.680	2	1	2	1	2
2	6.180	1	1	1	1	2
1	1.880	1	1	1	1	2
4	0.820	1	1	1	1	2
1	6.360	1	1	1	1	2
7	-0.470	2	1	1	1	2
2	6.240	1	1	1	1	2
2	-0.270	1	1	1	1	2
3	3.000	1	1	1	1	2
1	2.120	1	1	1	1	2
6	3.810	1	1	2	1	2
5	0.600	1	1	1	1	2
8	2.360	1	1	1	1	2
1	5.270	2	1	1	1	2
2	1.430	1	2	1	1	2
0	4.900	1	1	1	1	2
4	3.520	1	1	1	1	2
3	-0.210	1	1	1	1	2

1	0.750	1	1	1	1	2
6	5.330	1	1	1	1	2
3	1.590	1	1	1	1	2
2	2.200	1	1	1	1	2
7	1.660	1	1	1	1	2
0	3.920	1	1	1	1	2
2	1.150	1	1	1	1	2
8	2.750	2	1	1	1	2
1	2.060	1	1	1	1	2
3	3.180	1	1	1	1	2
3	4.280	1	1	1	1	2
2	3.560	1	1	1	1	2
6	4.100	1	1	1	1	2
6	1.560	1	1	1	1	2
1	3.500	2	1	1	1	2
2	4.410	1	1	1	1	2
1	2.830	1	1	1	1	2
1	4.210	1	1	1	1	2
5	6.200	1	1	1	1	2
7	6.200	1	1	1	1	2

#IUPAC	Compound	Y (log K <sub>OW</sub> exp)	Dipole (Debye)
CBz-00	benzene	2.13	0.00
CBz-01	1-chlorobenzene	2.98	1.80
BBz-01	1-bromobenzene	2.99	1.78
CBz-04	1,4-dichlorobenzene	3.44	0.00
CBz-03	1,3-dichlorobenzene	3.53	1.63
BBz-02	1,2-dibromobenzene	3.64	2.46
PCN-00	naphtalene	3.33	0.00
BBz-04	1,4-dibromobenzene	3.79	0.00
BBz-03	1,3-dibromobenzene	3.75	1.57
CBz-06	1,2,4-trichlorobenzene	4.02	1.23
CBz-07	1,3,5-trichlorobenzene	4.19	0.00
PCN-01	1-chloronaphtalene	3.90	1.67
PCN-02	2-chloronaphtalene	3.98	2.02
BBz-06	1,2,4-tribromobenzene	4.51	1.19
CBz-10	1,2,4,5-tetrachlorobenzene	4.70	0.00
CBz-09	1,2,3,5-tetrachlorobenzene	4.66	0.88
BBz-07	1,3,5-tribromobenzene	4.51	0.00
PCN-09	1,8-dichloronaphtalene	4.19	2.87
PCB-000	biphenyl	3.90	0.00
PCN-03	1,2-dichloronaphtalene	4.42	2.75
PCN-05	1,4-dichloronaphtalene	4.66	0.80
PCN-10	2,3-dichloronaphtalene	4.51	2.92
PCN-08	1,7-dichloronaphtalene	4.56	2.73
PCDD-00	dibenzo-p-dioxin	4.30	0.00
PCN-12	2,7-dichloronaphtalene	4.56	1.79
PCB-001	2-chlorobiphenyl	4.30	1.54
PBB-001	2-bromobiphenyl	4.59	1.55
PCB-002	3-chlorobiphenyl	4.60	1.94
CBz-12	1,2,3,4,5,6-hexachlorobenzene	5.73	0.00
PCN-26	2,3,6-trichloronaphtalene	5.12	1.42
PCN-21	1,3,7-trichloronaphtalene	5.35	1.42
PCDD-01	1-chlorodibenzo-p-dioxin	4.75	1.34
PBB-003	4-bromobiphenyl	4.96	2.01
PCB-004	2,2'-dichlorobiphenyl	4.90	1.53
PCB-010	2,6-dichlorobiphenyl	5.00	1.08
PCDE-001	2-chlorodiphenylether	4.45	2.55
PCDE-002	3-chlorodiphenylether	4.75	2.92
PCB-008	2,4'-dichlorobiphenyl	5.10	2.90
PCN-28	1,2,3,5-tetrachloronaphtalene	5.77	2.41
PCN-43	1,3,5,8-tetrachloronaphtalene	5.76	1.16
PBDE-003	4-bromodiphenylether	5.42	2.14
PCN-47	1,4,6,7-tetrachloronaphtalene	5.81	1.89
PCDF-016	2,8-dichlorodibenzofuran	5.44	1.18
PCDE-010	2,6-dichlorodiphenylether	4.64	2.06
PCB-015	4,4'-dichlorobiphenyl	5.30	0.00
PCB-011	3,3'-dichlorobiphenyl	5.30	1.46
PCN-42	1,3,5,7-tetrachloronaphtalene	6.19	0.00
BBz-12	1,2,3,4,5,6-hexabromobenzene	6.07	0.00
PCDD-11	2,7-dichlorodibenzo-p-dioxin	6.38	0.00



PCB-030	2,4,6-trichlorobiphenyl	5.50	0.68
PCDE-008	2,4'-dichlorodiphenylether	5.03	2.63
PCDE-007	2,4-dichlorodiphenylether	4.93	2.63
PCDE-009	2,5-dichlorodiphenylether	5.13	1.42
PCB-029	2,4,5-trichlorobiphenyl	5.60	1.88
PCB-033	2,3',4'-trichlorobiphenyl	5.80	3.42
PBDE-008	2,4'-dibromodiphenylether	5.59	3.03
PCDE-015	4,4'-dichlorodiphenylether	5.25	0.08
PBB-015	4,4'-dibromobiphenyl	5.72	0.00
PCDE-013	3,4'-dichlorodiphenylether	5.13	1.58
PCB-054	2,6,2',6'-tetrachlorobiphenyl	5.48	0.00
PCDE-024	2,3,6-trichlorodiphenylether	5.35	2.20
PCB-037	3,4,4'-trichlorobiphenyl	5.90	1.37
PCDE-017	2,4,2'-trichlorodiphenylether	4.96	3.47
PCDE-032	2,6,4'-trichlorodiphenylether	5.30	3.06
PCDE-030	2,4,6-trichlorodiphenylether	5.32	1.35
PCB-053	2,5,2',6'-tetrachlorobiphenyl	5.50	1.60
PCB-040	2,3,2',3'-tetrachlorobiphenyl	5.60	2.45
PBB-030	2,4,6-tribromobiphenyl	6.03	0.69
PCDE-021	2,3,4-trichlorodiphenylether	5.55	3.79
PCB-061	2,3,4,5-tetrachlorobiphenyl	5.90	2.56
PCB-052	2,5,2',5'-tetrachlorobiphenyl	6.10	0.01
PCDE-022	2,3,4'-trichlorodiphenylether	5.63	2.50
PCB-049	2,4,2',5'-tetrachlorobiphenyl	6.10	1.50
PCDE-029	2,4,5-trichlorodiphenylether	5.58	2.48
PCDF-051	1,2,3,7-tetrachlorodibenzofuran	6.39	0.74
PCDE-023	2,3,5-trichlorodiphenylether	5.62	2.87
PCB-075	2,4,6,4'-tetrachlorobiphenyl	6.21	1.27
PCDE-025	2,4,3'-trichlorodiphenylether	5.65	1.47
PCDE-035	3,4,3'-trichlorodiphenylether	5.74	2.50
PCDE-031	2,5,4'-trichlorodiphenylether	5.66	0.91
PCB-066	2,4,3',4'-tetrachlorobiphenyl	5.80	1.83
PCDF-083	2,3,7,8-tetrachlorodibenzofuran	6.53	0.09
PCDE-039	3,5,4'-trichlorodiphenylether	5.77	0.66
PCDE-062	2,3,4,6-tetrachlorodiphenylether	5.88	2.13
PCDE-041	2,3,4,2'-tetrachlorodiphenylether	5.72	4.56
PCDE-065	2,3,5,6-tetrachlorodiphenylether	5.82	1.58
PCB-068	2,4,3',5'-tetrachlorobiphenyl	6.20	1.50
PBDE-030	2,4,6-tribromodiphenylether	6.20	1.41
PBDE-032	2,6,4'-tribromodiphenylether	6.20	3.10
PCB-077	3,4,3',4'-tetrachlorobiphenyl	6.50	1.17
PCDE-071	2,6,3',4'-tetrachlorodiphenylether	5.70	3.11
PCB-116	2,3,4,5,6-pentachlorobiphenyl	6.30	1.78
PCDE-064	2,3,6,4'-tetrachlorodiphenylether	5.64	2.17
PCDD-27	1,2,3,4-tetrachlorodibenzo-p-dioxin	6.60	3.01
PCDE-049	2,4,2',5'-tetrachlorodiphenylether	5.78	2.32
PCB-087	2,3,4,2',5'-pentachlorobiphenyl	6.50	2.45
PCDD-29	1,2,3,7-tetrachlorodibenzo-p-dioxin	6.90	1.21
PCB-110	2,3,6,3',4'-pentachlorobiphenyl	6.30	2.77
PCDE-061	2,3,4,5-tetrachlorodiphenylether	6.01	3.50

PCDD-48	2,3,7,8-tetrachlorodibenzo-p-dioxin	6.80	0.00
PCDE-056	2,3,3',4'-tetrachlorodiphenylether	5.99	2.21
PCDE-055	2,3,4,3'-tetrachlorodiphenylether	6.07	2.54
PCDE-060	2,3,4,4'-tetrachlorodiphenylether	6.14	2.02
PCDE-091	2,3,6,2',4'-pentachlorodiphenylether	6.06	1.82
PCB-105	2,3,4,3',4'-pentachlorobiphenyl	6.00	1.89
PBDE-037	3,4,4'-tribromodiphenylether	6.02	1.47
PCDD-42	1,3,6,8-tetrachlorodibenzo-p-dioxin	7.18	0.00
PCDE-081	3,4,5,4'-tetrachlorodiphenylether	6.30	1.65
PCDE-066	2,4,3',4'-tetrachlorodiphenylether	6.13	1.38
PCDE-070	2,5,3',4'-tetrachlorodiphenylether	6.11	1.61
PCDE-077	3,4,3',4'-tetrachlorodiphenylether	6.36	1.41
PBB-052	2,5,2',5'-tetrabromobiphenyl	6.50	0.14
PCB-136	2,3,6,2',3',6'-hexachlorobiphenyl	6.70	1.35
PBDF-061	1,2,7,8-tetrabromodibenzofuran	6.20	1.94
PCDE-067	2,4,5,3'-tetrachlorodiphenylether	6.14	1.69
PCDE-063	2,3,5,4'-tetrachlorodiphenylether	6.21	1.11
PCDF-114	2,3,4,7,8-pentachlorodibenzofuran	6.5	0.83
PCDE-100	2,4,6,2',4'-pentachlorodiphenylether	6.11	0.74
PCDE-089	2,3,4,2',6'-pentachlorodiphenylether	6.11	4.72
PBDE-047	2,4,2',4'-tetrabromodiphenylether	6.86	0.84
PCDE-082	2,3,4,2',3'-pentachlorodiphenylether	6.30	3.85
PCDE-102	2,4,5,2',6'-pentachlorodiphenylether	5.98	3.31
PCB-134	2,3,5,6,2',3'-hexachlorobiphenyl	7.30	2.30
PBDF-083	2,3,7,8-tetrabromodibenzofuran	5.98	0.00
PCDE-109	2,3,4,6,3'-pentachlorodiphenylether	6.58	1.22
PCDE-097	2,3,2',4',5'-pentachlorodiphenylether	6.22	2.70
PCDE-087	2,3,4,2',5'-pentachlorodiphenylether	6.51	3.31
PCDE-115	2,3,4,6,4'-pentachlorodiphenylether	6.47	1.01
PCDE-085	2,3,4,2',4'-pentachlorodiphenylether	6.28	2.88
PCDE-117	2,3,5,6,4'-pentachlorodiphenylether	6.41	0.99
PCB-128	2,3,4,2',3',4'-hexachlorobiphenyl	7.00	2.10
PCDE-101	2,4,5,2',5'-pentachlorodiphenylether	6.22	1.82
PCDE-099	2,4,5,2',4'-pentachlorodiphenylether	6.38	1.66
PCDE-119	2,4,6,3',4'-pentachlorodiphenylether	6.44	1.66
PCDE-123	2,4,3',4',5'-pentachlorodiphenylether	6.63	2.60
PCDE-090	2,3,5,2',4'-pentachlorodiphenylether	6.54	1.88
PCDD-50	1,2,3,4,7-pentachlorodibenzo-p-dioxin	7.40	1.44
PCB-153	2,4,5,2',4',5'-hexachlorobiphenyl	6.90	0.16
PCDE-114	2,3,4,5,4'-pentachlorodiphenylether	6.61	1.56
PCDE-139	2,3,4,6,2',4'-hexachlorodiphenylether	6.84	1.51
PCDE-147	2,3,5,6,2',4'-hexachlorodiphenylether	6.76	0.82
PCDE-108	2,3,4,3',5'-pentachlorodiphenylether	6.52	1.73
PCDE-126	3,4,5,3',4'-pentachlorodiphenylether	6.83	1.77
PCDE-132	2,3,4,2',3',6'-hexachlorodiphenylether	6.47	3.74
PCDE-166	2,3,4,5,6,4'-hexachlorodiphenylether	6.95	0.20
PCDE-128	2,3,4,2',3',4'-hexachlorodiphenylether	6.82	2.70
PBB-101	2,4,5,2',5'-pentabromobiphenyl	7.10	1.29
PBDF-094	1,2,3,7,8-pentabromodibenzofuran	7.04	0.79
PBDE-077	3,4,3',4'-tetrabromodiphenylether	6.86	1.36

PCB-185	2,3,4,5,6,2',5'-heptachlorobiphenyl	7.00	1.18
PCB-171	2,3,4,6,2',3',4'-heptachlorobiphenyl	6.70	2.19
PCDE-140	2,3,4,2',4',6'-hexachlorodiphenylether	6.65	3.09
PCDE-163	2,3,5,6,3',4'-hexachlorodiphenylether	6.78	1.36
PCDE-137	2,3,4,5,2',4'-hexachlorodiphenylether	6.72	2.50
PCDE-138	2,3,4,2',4',5'-hexachlorodiphenylether	7.01	2.21
PCDE-130	2,3,4,2',3',5'-hexachlorodiphenylether	7.01	2.48
PCDE-154	2,4,5,2',4',6'-hexachlorodiphenylether	6.49	1.62
PBDE-099	2,4,5,2',4'-pentabromodiphenylether	7.17	1.18
PCDE-146	2,3,5,2',4',5'-hexachlorodiphenylether	6.76	1.25
PCDE-181	2,3,4,5,6,2',4'-heptachlorodiphenylether	7.31	1.30
PCDE-157	2,3,4,3',4',5'-hexachlorodiphenylether	6.99	1.78
PCDE-156	2,3,4,5,3',4'-hexachlorodiphenylether	7.07	1.37
PCDE-187	2,3,5,6,2',4',5'-heptachlorodiphenylether	7.13	1.02
PCDE-167	2,4,5,3',4',5'-hexachlorodiphenylether	7.11	1.27
PCB-202	2,3,5,6,2',3',5',6'-octachlorobiphenyl	7.10	0.00
PCDE-174	2,3,4,5,2',3',6'-heptachlorodiphenylether	6.98	3.37
PCDE-170	2,3,4,5,2',3',4'-heptachlorodiphenylether	7.28	2.43
PCDE-180	2,3,4,5,2',4',5'-heptachlorodiphenylether	7.46	1.55
PCB-194	2,3,4,5,2',3',4',5'-octachlorobiphenyl	7.40	0.89
PCDE-195	2,3,4,5,6,2',3',4'-octachlorodiphenylether	7.84	1.57
PCDE-203	2,3,4,5,6,2',4',5'-octachlorodiphenylether	7.81	0.43
PCB-208	2,3,4,5,6,2',3',5',6'-nonachlorobiphenyl	8.16	0.84
PCDE-189	2,3,4,5,3',4',5'-heptachlorodiphenylether	7.55	0.54
PCB-207	2,3,4,5,6,2',3',4',6'-nonachlorobiphenyl	7.52	0.88
PCDD-75	1,2,3,4,6,7,8,9-octachlorodibenzo-p-dioxin	8.20	0.00
PCB-209	2,3,4,5,6,2',3',4',5',6'-decachlorobiphenyl	8.26	0.00
PCDE-209	2,3,4,5,6,2',3',4',5',6'-decachlorodiphenylether	8.16	0.44
PBB-209	2,3,4,5,6,2',3',4',5',6'-decabromobiphenyl	8.50	0.00
CBz-02	1,2-dichlorobenzene	3.43	2.52
CBz-05	1,2,3-trichlorobenzene	4.14	2.51
CBz-08	1,2,3,4-tetrachlorobenzene	4.64	1.85
PCDF-000	dibenzofuran	4.27	1.18
PCN-06	1,5-dichloronaphtalene	4.67	0.00
CBz-11	1,2,3,4,5-pentachlorobenzene	5.18	0.83
PCDE-000	diphenylether	3.97	1.27
BBz-10	1,2,4,5-tetrabromobenzene	5.13	0.00
PCB-003	4-chlorobiphenyl	4.50	1.98
PBB-002	3-bromobiphenyl	4.85	1.92
PCDD-02	2-chlorodibenzo-p-dioxin	5.00	1.97
PCN-27	1,2,3,4-tetrachloronaphtalene	5.75	2.89
PCDE-003	4-chlorodiphenylether	4.70	2.03
PCB-009	2,5-dichlorobiphenyl	5.10	0.57
PCB-007	2,4-dichlorobiphenyl	5.00	1.82
PCB-018	2,5,2'-trichlorobiphenyl	5.60	1.84
PCDE-005	2,3-dichlorodiphenylether	5.00	3.61
PCDE-012	3,4-dichlorodiphenylether	4.99	3.49
PCDE-014	3,5-dichlorodiphenylether	5.21	2.57
PBDE-007	2,4-dibromodiphenylether	5.83	1.28
PCB-044	2,3,2',5'-tetrachlorobiphenyl	6.00	2.41

PCDE-038	3,4,5-trichlorodiphenylether	5.70	3.46
PCDE-033	2,3',4'-trichlorodiphenylether	5.50	2.73
PCB-047	2,4,2',4'-tetrachlorobiphenyl	5.90	1.38
PCB-060	2,3,4,4'-tetrachlorobiphenyl	6.31	2.01
PCDE-037	3,4,4'-trichlorodiphenylether	5.88	1.52
PCDE-028	2,4,4'-trichlorodiphenylether	5.53	1.17
PCB-088	2,3,4,6,2'-pentachlorobiphenyl	6.50	2.39
PCDE-048	2,4,5,2'-tetrachlorodiphenylether	5.97	3.28
PCDE-042	2,3,2',4'-tetrachlorodiphenylether	5.88	2.84
PCDE-047	2,4,2',4'-tetrachlorodiphenylether	5.95	1.90
PCDE-075	2,4,6,4'-tetrachlorodiphenylether	5.92	1.30
PCB-101	2,4,5,2',5'-pentachlorobiphenyl	6.40	1.29
PCDE-074	2,4,5,4'-tetrachlorodiphenylether	5.99	0.52
PCDE-068	2,4,3',5'-tetrachlorodiphenylether	6.13	1.69
PCN-75	1,2,3,4,5,6,7,8-octachloronaphtalene	6.42	0.00
PCDE-116	2,3,4,5,6-pentachlorodiphenylether	6.37	2.06
PCDE-079	3,4,3',5'-tetrachlorodiphenylether	6.22	1.04
PCDE-110	2,3,6,3',4'-pentachlorodiphenylether	6.31	2.15
PCB-155	2,4,6,2',4',6'-hexachlorobiphenyl	7.00	0.00
PCB-129	2,3,4,5,2',3'-hexachlorobiphenyl	7.30	2.77
PCDF-118	1,2,3,4,7,8-hexachlorodibenzofuran	7	0.08
PCDE-105	2,3,4,3',4'-pentachlorodiphenylether	6.51	1.66
PCDE-149	2,3,6,2',4',5'-hexachlorodiphenylether	6.47	2.19
PBDD-48	2,3,7,8-tetrabromodibenzo-p-dioxin	6.50	0.00
PCDE-118	2,4,5,3',4'-pentachlorodiphenylether	6.60	1.13
PCDE-120	2,4,5,3',5'-pentachlorodiphenylether	6.66	0.34
PBB-155	2,4,6,2',4',6'-hexabromobiphenyl	7.20	0.00
PCDE-153	2,4,5,2',4',5'-hexachlorodiphenylether	6.72	0.56
PCDD-66	1,2,3,4,7,8-hexachlorodibenzo-p-dioxin	7.80	0.10
PCDF-131	1,2,3,4,6,7,8-heptachlorodibenzofuran	7.4	0.78
PCDE-177	2,3,4,2',3',5',6'-heptachlorodiphenylether	7.14	2.81
PCDE-190	2,3,4,5,6,3',4'-heptachlorodiphenylether	7.31	1.02
PCDF-135	1,2,3,4,6,7,8,9-octachlorodibenzofuran	8	0.08
PCDD-73	1,2,3,4,6,7,8-heptachlorodibenzo-p-dioxin	8.00	0.70
PCDE-199	2,3,4,5,2',3',5',6'-octachlorodiphenylether	7.63	2.28
PCB-206	2,3,4,5,6,2',3',4',5'-nonachlorobiphenyl	7.20	0.99
PCDE-194	2,3,4,5,2',3',4',5'-octachlorodiphenylether	7.78	1.26
PCDE-206	2,3,4,5,6,2',3',4',5'-nonachlorodiphenylether	8.07	0.53

(A3)	Z to 1	(kX)	(Y/kX)	(kY/kX)	Duplex
120.13	1	1	1	1	1
138.85	2	1	1	1	1
144.46	1	1	1	1	1
158.13	2	2	1	1	1
158.14	1	2	1	1	1
164.96	1	1	1	1	1
167.06	1	1	1	1	1
169.13	2	2	1	1	1
169.39	1	2	1	1	1
174.54	1	1	1	1	1
177.66	1	1	1	1	1
182.86	1	1	1	1	1
185.96	2	2	1	1	1
189.45	1	1	1	1	1
190.63	1	1	1	1	1
191.24	2	1	1	1	1
193.89	2	1	1	1	1
196.18	2	1	1	1	1
198.47	1	1	1	1	1
199.10	2	1	1	1	1
199.13	1	1	1	2	1
201.79	1	2	1	1	1
202.35	1	2	2	2	1
204.83	1	1	1	1	1
205.09	1	1	1	1	1
211.19	1	1	1	1	1
215.59	2	1	1	1	1
217.53	1	2	1	1	1
217.89	1	1	1	1	1
221.06	2	2	1	1	1
221.56	2	1	2	2	1
222.93	1	1	1	1	1
223.03	1	1	2	2	1
223.69	2	2	2	2	1
224.24	1	1	1	1	1
226.72	1	1	1	1	1
228.15	1	2	1	1	1
230.52	1	1	1	1	1
231.35	2	1	1	1	1
231.49	1	1	1	1	1
233.18	1	1	1	1	1
234.46	2	1	1	1	1
234.50	1	1	2	1	1
235.12	1	1	1	1	1
236.35	2	1	1	1	1
236.76	1	1	1	1	1
237.79	1	2	1	1	1
242.82	1	2	2	2	1
243.04	2	1	1	1	1

243.29	2	1	1	1	1
244.45	1	1	1	1	1
245.37	1	1	1	1	1
245.73	1	1	1	1	1
246.81	2	1	1	2	1
246.91	1	1	2	2	1
247.44	1	1	1	1	1
247.57	1	2	1	1	1
247.58	1	1	2	2	1
247.88	1	2	1	1	1
248.54	1	2	1	1	1
251.55	1	1	1	1	1
252.87	1	2	1	1	1
254.28	1	1	1	1	1
254.38	1	1	2	2	1
254.76	1	2	1	1	1
256.15	1	1	1	1	1
256.24	1	1	1	1	1
257.79	2	1	1	1	1
258.62	2	2	1	1	1
260.27	2	1	2	2	1
260.74	1	1	1	1	1
261.32	1	2	1	1	1
261.55	2	1	1	1	1
261.76	1	1	2	2	1
261.97	1	1	2	2	1
262.36	1	1	1	1	1
262.41	1	1	1	1	1
263.50	1	1	1	1	1
264.20	2	1	1	1	1
264.39	1	2	1	1	1
266.02	1	1	1	1	1
266.62	2	1	1	1	1
266.67	1	1	1	1	1
268.01	1	2	1	2	1
268.32	1	1	1	1	1
268.54	1	1	2	1	1
268.56	1	1	1	2	1
268.70	1	1	2	2	1
268.73	1	2	1	1	1
269.33	1	1	1	1	1
269.85	2	2	1	1	1
270.01	1	1	1	1	1
270.69	2	1	1	1	1
271.19	1	1	1	1	1
273.50	1	1	1	1	1
274.92	1	2	1	1	1
275.01	1	2	1	1	1
275.05	2	1	2	2	1
275.60	1	2	1	1	1

276.24	2	2	1	1	1
277.28	1	2	2	2	1
277.60	1	1	1	1	1
277.82	1	2	2	2	1
278.66	1	1	1	1	1
279.26	1	1	2	2	1
279.43	1	1	2	2	1
279.76	1	1	1	1	1
279.98	1	1	2	2	1
280.09	1	2	1	1	1
280.55	1	2	2	2	1
280.66	1	1	2	2	1
280.71	1	1	1	1	1
280.74	1	2	2	1	1
280.80	2	1	1	1	1
281.16	2	1	2	2	1
281.52	1	1	2	2	1
281.84	2	1	2	2	1
281.93	2	1	1	1	1
282.87	1	1	1	1	1
284.22	2	1	1	1	1
284.30	1	2	1	1	1
285.36	1	1	1	1	1
285.67	1	1	1	1	1
286.10	2	1	1	1	1
286.39	1	1	1	1	1
286.82	1	2	2	2	1
286.84	1	2	2	2	1
287.09	1	2	2	2	1
287.37	1	2	1	1	1
287.39	2	1	1	1	1
288.54	1	2	2	2	1
288.96	1	2	1	1	1
289.34	1	1	2	2	1
289.39	1	1	2	2	1
289.55	1	1	1	1	1
289.98	1	1	1	2	1
290.31	1	1	1	1	1
293.63	1	1	2	2	1
294.81	1	1	2	2	1
294.96	1	1	1	1	1
295.71	1	1	1	1	1
296.51	1	2	2	2	1
296.54	1	2	1	1	1
299.63	2	1	1	1	1
300.59	2	1	2	2	1
300.66	1	1	1	1	1
301.00	1	2	2	2	1
301.08	1	1	1	1	1
301.24	1	1	2	2	1

302.02	1	2	2	2	1
302.07	1	1	1	1	1
302.40	1	2	1	1	1
302.72	1	2	1	1	1
303.12	1	1	2	2	1
303.24	2	1	2	2	1
303.65	1	1	1	1	1
304.73	1	1	1	1	1
305.12	2	2	2	1	1
305.94	1	1	1	1	1
308.61	1	1	1	1	1
309.73	1	1	1	1	1
310.92	1	1	1	1	1
311.48	1	1	2	2	1
312.86	1	2	1	1	1
313.15	2	1	1	1	1
315.18	1	2	1	1	1
316.62	2	2	1	1	1
318.95	2	1	1	1	1
320.58	1	2	1	1	1
321.76	1	1	1	1	1
324.41	1	2	1	1	1
326.99	1	2	2	1	1
327.11	1	1	1	1	1
327.18	1	1	2	2	1
332.09	1	1	1	1	1
340.62	1	1	1	1	1
350.17	2	1	1	1	1
366.58	1	1	1	1	1
155.23	1	1	1	1	2
171.70	1	1	1	1	2
188.21	1	1	1	1	2
195.76	1	1	1	1	2
199.29	1	1	1	1	2
204.50	2	2	1	1	2
209.13	1	1	1	1	2
210.22	1	1	1	1	2
217.08	1	1	2	2	2
222.93	1	1	2	2	2
224.07	1	1	1	1	2
228.03	1	1	1	1	2
228.37	2	1	1	1	2
230.17	1	1	1	1	2
230.36	1	1	1	1	2
241.87	1	1	1	1	2
242.48	2	1	1	1	2
244.32	2	1	1	1	2
247.09	1	1	2	2	2
247.34	1	1	1	1	2
258.72	2	1	1	1	2



260.34	1	1	2	2	2
260.50	1	1	1	1	2
261.95	1	1	2	2	2
263.10	2	1	1	1	2
263.62	1	1	2	2	2
264.30	1	1	2	2	2
269.35	1	2	1	1	2
270.08	1	1	2	2	2
271.19	2	1	2	1	2
273.66	1	1	2	2	2
274.08	1	1	1	1	2
277.22	1	1	1	1	2
281.22	1	1	2	2	2
281.28	1	1	2	2	2
281.45	1	1	2	2	2
281.69	1	1	1	1	2
282.84	2	1	1	1	2
286.57	1	1	1	1	2
286.94	2	1	1	1	2
288.39	1	1	1	1	2
293.46	1	2	1	1	2
293.80	1	1	1	1	2
294.85	1	1	2	1	2
295.58	2	2	1	1	2
297.49	2	1	1	1	2
299.60	2	1	1	1	2
303.56	1	1	1	1	2
305.36	2	1	1	1	2
306.74	1	2	1	1	2
309.25	1	2	1	2	2
315.87	1	1	1	2	2
316.37	2	1	1	1	2
318.13	1	1	1	1	2
319.40	2	1	1	1	2
331.48	1	1	1	1	2
331.76	1	1	1	1	2
332.50	2	1	1	1	2
338.02	1	1	1	1	2

#IUPAC	Compound	Y (log K <sub>OA</sub> exp)	Energy of HOMO (eV)	Mean polarizability (Å <sup>3</sup> )
CBz-03	1,3-dichlorobenzene	4.25	-9.75	14.44
CBz-05	1,2,3-trichlorobenzene	5.06	-9.74	16.49
CBz-08	1,2,3,4-tetrachlorobenzene	5.73	-9.71	18.79
PCB-187	2,3,5,6,2',4',5'-heptachlorobiphenyl	9.87	-9.69	36.21
PCB-180	2,3,4,5,2',4',5'-heptachlorobiphenyl	9.88	-9.65	36.57
CBz-00	benzene	2.80	-9.64	10.16
PCB-149	2,3,6,2',4',5'-hexachlorobiphenyl	9.27	-9.63	33.76
CBz-06	1,2,4-trichlorobenzene	4.93	-9.62	16.69
PBDE-153	2,4,5,2',4',5'-hexabromodiphenylether	11.82	-9.62	42.55
CBz-10	1,2,4,5-tetrachlorobenzene	5.57	-9.62	18.96
PBDE-126	3,4,5,3',4'-pentabromodiphenylether	11.97	-9.59	39.21
PCB-095	2,3,6,2',5'-pentachlorobiphenyl	8.71	-9.58	31.26
PBDE-154	2,4,5,2',4',6'-hexabromodiphenylether	11.92	-9.58	42.36
PCB-153	2,4,5,2',4',5'-hexachlorobiphenyl	9.80	-9.56	34.31
CBz-04	1,4-dichlorobenzene	4.27	-9.55	14.50
PCB-044	2,3,2',5'-tetrachlorobiphenyl	8.36	-9.54	29.02
PCB-110	2,3,6,3',4'-pentachlorobiphenyl	9.06	-9.52	31.62
PCB-077	3,4,3',4'-tetrachlorobiphenyl	9.29	-9.49	29.93
PBDE-077	3,4,3',4'-tetrabromodiphenylether	10.87	-9.48	35.82
PCB-061	2,3,4,5-tetrachlorobiphenyl	8.80	-9.48	29.63
PCB-064	2,3,6,4'-tetrachlorobiphenyl	8.41	-9.47	29.40
PCN-67	1,2,3,5,6,7-hexachloronaphtalene	9.70	-9.47	31.41
PBDE-085	2,3,4,2',4'-pentabromodiphenylether	11.66	-9.47	38.44
PBDE-100	2,4,6,2',4'-pentabromodiphenylether	11.13	-9.45	38.69
PCN-66	1,2,3,4,6,7-hexachloronaphtalene	9.70	-9.44	31.47
PCB-018	2,5,2'-trichlorobiphenyl	7.60	-9.42	26.81
PCN-52	1,2,3,5,7-pentachloronaphtalene	8.73	-9.41	28.92
PCN-70	1,2,3,6,7,8-hexachloronaphtalene	9.89	-9.39	31.39
PCN-60	1,2,4,6,7-pentachloronaphtalene	8.73	-9.38	28.97
PBDE-047	2,4,2',4'-tetrabromodiphenylether	10.53	-9.38	35.19
PCB-029	2,4,5-trichlorobiphenyl	8.01	-9.37	27.41
PCN-50	1,2,3,4,6-pentachloronaphtalene	8.91	-9.34	28.92
PCN-47	1,4,6,7-tetrachloronaphtalene	8.13	-9.33	26.37
PCN-68	1,2,3,5,6,8-hexachloronaphtalene	9.80	-9.32	31.22
PCN-64	1,2,3,4,5,7-hexachloronaphtalene	9.80	-9.32	31.25
PCN-34	1,2,4,7-tetrachloronaphtalene	8.08	-9.31	26.51
PCN-58	1,2,4,5,7-pentachloronaphtalene	8.86	-9.30	28.84
PCN-25	1,6,7-trichloronaphtalene	7.54	-9.30	24.07
PCN-69	1,2,3,5,7,8-hexachloronaphtalene	9.83	-9.29	31.17
PCN-28	1,2,3,5-tetrachloronaphtalene	8.26	-9.29	26.25
PBDE-013	3,4'-dibromodiphenylether	8.57	-9.29	28.99
PBDE-017	2,4,2'-tribromodiphenylether	9.30	-9.27	31.41
PCN-17	1,2,7-trichloronaphtalene	7.54	-9.26	24.14
PCN-33	1,2,4,6-tetrachloronaphtalene	8.08	-9.25	26.50
PBDE-028	2,4,4'-tribromodiphenylether	9.50	-9.25	32.09
PCN-63	1,2,3,4,5,6-hexachloronaphtalene	10.11	-9.25	31.11
PBDE-012	3,4-dibromodiphenylether	8.55	-9.25	28.76
PCN-53	1,2,3,5,8-pentachloronaphtalene	9.13	-9.24	28.57
PCN-61	1,2,4,6,8-pentachloronaphtalene	8.78	-9.23	28.79

PCB-003	4-chlorobiphenyl	6.80	-9.23	23.02
PCN-13	1,2,3-trichloronaphthalene	7.62	-9.23	24.05
PCN-19	1,3,5-trichloronaphthalene	7.32	-9.22	23.94
PCN-16	1,2,6-trichloronaphthalene	7.50	-9.22	24.20
PCN-24	1,4,6-trichloronaphthalene	7.27	-9.21	24.00
PBDE-015	4,4'-dibromodiphenylether	8.64	-9.21	29.00
PCN-62	1,2,4,7,8-pentachloronaphthalene	9.06	-9.20	28.66
PCN-57	1,2,4,5,6-pentachloronaphthalene	9.15	-9.20	28.72
PCN-27	1,2,3,4-tetrachloronaphthalene	8.33	-9.19	26.29
PBDE-002	3-bromodiphenylether	7.36	-9.19	25.28
PCN-15	1,2,5-trichloronaphthalene	7.45	-9.17	23.87
PCDD-73	1,2,3,4,6,7,8-heptachlorodibenzo-p-dioxin	11.42	-9.17	39.04
PBDE-007	2,4-dibromodiphenylether	8.37	-9.16	28.41
PCN-65	1,2,3,4,5,8-hexachloronaphthalene	10.37	-9.14	30.99
PCN-32	1,2,4,5-tetrachloronaphthalene	8.58	-9.14	26.22
PCN-35	1,2,4,8-tetrachloronaphthalene	8.41	-9.10	26.15
PCN-59	1,2,4,5,8-pentachloronaphthalene	9.18	-9.09	28.57
PBDE-010	2,6-dibromodiphenylether	8.12	-9.09	27.99
PCN-02	2-chloronaphthalene	5.76	-9.08	19.60
PCN-06	1,5-dichloronaphthalene	6.62	-9.07	21.46
PCN-03	1,2-dichloronaphthalene	6.76	-9.07	21.65
PCN-05	1,4-dichloronaphthalene	6.93	-9.04	21.54
PCDD-50	1,2,3,4,7-pentachlorodibenzo-p-dioxin	10.67	-9.03	34.34
PCN-46	1,4,5,8-tetrachloronaphthalene	8.45	-9.01	26.08
PCDE-000	diphenylether	6.42	-8.92	21.63
PCDD-27	1,2,3,4-tetrachlorodibenzo-p-dioxin	9.70	-8.89	31.63
PCDD-11	2,7-dichlorodibenzo-p-dioxin	8.36	-8.78	27.41
PCDD-01	1-chlorodibenzo-p-dioxin	7.86	-8.60	24.45
CBz-07	1,3,5-trichlorobenzene	4.77	-10.06	16.79
CBz-12	1,2,3,4,5,6-hexachlorobenzene	6.77	-9.83	23.52
CBz-09	1,2,3,5-tetrachlorobenzene	5.56	-9.74	18.95
CBz-11	1,2,3,4,5-pentachlorobenzene	6.13	-9.73	21.21
CBz-02	1,2-dichlorobenzene	4.40	-9.57	14.29
PBDE-156	2,3,4,5,3',4'-hexabromodiphenylether	11.97	-9.56	42.36
PCB-101	2,4,5,2',5'-pentachlorobiphenyl	9.14	-9.54	31.76
PCB-052	2,5,2',5'-tetrachlorobiphenyl	8.22	-9.52	29.21
PBDE-099	2,4,5,2',4'-pentabromodiphenylether	11.31	-9.50	38.90
PBDE-066	2,4,3',4'-tetrabromodiphenylether	10.82	-9.41	35.34
PCN-73	1,2,3,4,5,6,7-heptachloronaphthalene	10.63	-9.36	33.73
PCN-37	1,2,5,7-tetrachloronaphthalene	8.08	-9.34	26.45
PCN-12	2,7-dichloronaphthalene	6.66	-9.34	22.09
PCB-015	4,4'-dichlorobiphenyl	7.73	-9.31	25.46
PCN-75	1,2,3,4,5,6,7,8-octachloronaphthalene	11.48	-9.27	36.13
PCN-72	1,2,4,5,7,8-hexachloronaphthalene	9.89	-9.18	31.13
PBDE-008	2,4'-dibromodiphenylether	8.47	-9.11	28.28
PCDD-66	1,2,3,4,7,8-hexachlorodibenzo-p-dioxin	11.11	-9.09	36.91
PCN-23	1,4,5-trichloronaphthalene	7.56	-9.04	23.74
PCDD-54	1,2,3,7,8-pentachlorodibenzo-p-dioxin	10.57	-9.02	34.64
PBDE-001	2-bromodiphenylether	7.24	-9.01	24.63
PCN-01	1-chloronaphthalene	5.81	-8.98	19.29

PCDD-48	2,3,7,8-tetrachlorodibenzo-p-dioxin	10.05	-8.94	32.43
PCN-00	naphtalene	5.19	-8.88	17.21
PCDD-26	2,3,7-trichlorodibenzo-p-dioxin	9.14	-8.86	29.87
PCDD-12	2,8-dichlorodibenzo-p-dioxin	8.36	-8.77	27.30

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CAS	Y (logER-RBA exp)	Average Information content (order 1)	Number of rings
106-44-5	-4.5	2.58	1
123-07-9	-4.17	2.6	1
153-18-4	-4.09	3.66	5
620-17-7	-3.87	2.79	1
6640-27-3	-3.66	3.11	1
89-72-5	-3.54	2.78	1
103-16-2	-3.44	2.42	2
580-51-8	-3.44	1.96	2
99-76-3	-3.44	3.05	1
59-50-7	-3.38	2.98	1
80-46-6	-3.26	2.71	1
143-74-8	-3.25	2.75	4
120-47-8	-3.22	3.11	1
94-13-3	-3.22	3.14	1
126-00-1	-3.13	3.2	2
480-16-0	-3.09	3.06	3
80-09-1	-3.07	3.07	1
94-26-8	-3.07	2.61	2
92-69-3	-3.04	1.96	2
620-92-8	-3.02	2.61	2
521-18-6	-2.89	2.13	4
13037-86-0	-2.88	2.61	1
789-02-6	-2.85	2.71	2
94-41-7	-2.82	1.94	2
58-72-0	-2.78	1.63	3
6335-83-7	-2.69	2.48	2
131-56-6	-2.61	2.55	2
94-18-8	-2.54	2.82	2
97-23-4	-2.45	3.09	2
2657-25-2	-2.43	2.42	2
528-48-3	-2.35	3.05	3
1806-26-4	-2.31	2.43	1
599-64-4	-2.3	2.46	2
80-05-7	-2.11	2.82	2
1085-12-7	-2.09	2.88	1
143-50-0	-1.89	1.98	5
77-09-8	-1.87	2.7	4
140-66-9	-1.82	2.48	1
5153-25-3	-1.74	2.93	1
104-43-8	-1.73	2.24	1
486-66-8	-1.65	2.98	3
520-18-3	-1.61	3.05	3
500-38-9	-1.51	3.05	2
603-45-2	-1.5	2.56	3
68-23-5	-0.67	2.87	4
2971-36-0	-0.6	2.88	2
659-22-3	-0.55	2.41	2
446-72-0	-0.36	3.08	3
2529-64-8	-0.3	2.68	4



1229-24-9	-0.15	3.12	4
479-13-0	-0.05	3.13	4
72-33-3	0.35	3.22	4
50-28-2	0.49	3.01	4
53-16-7	0.86	3	4
50-27-1	0.99	3.15	4
53-63-4	1.14	2.74	4
129453-61-8	1.16	2.64	4
362-05-0	1.47	3.07	4
84-17-3	1.57	2.97	2
68047-06-3	2.24	3	3
57-63-6	2.28	3.3	4
56-53-1	2.6	2.94	2
1570-64-5	-3.67	3.11	1
98-54-4	-3.61	2.53	1
99-71-8	-3.37	2.7	1
92-04-6	-2.77	2.26	2
20426-12-4	-2.55	2.33	2
520-36-5	-1.55	3.08	3

Relative ALFA polarizability (DIP) (AM1)	Max net atomic charge (Zefirov) for O atoms	logP	Z to 1
0.61	-0.17	2.06	1
0.58	-0.17	2.55	1
0.62	-0.11	-1.11	1
0.56	-0.17	2.55	1
0.59	-0.17	2.7	1
0.55	-0.17	3.46	1
0.63	-0.17	3.3	1
0.69	-0.17	3.19	1
0.6	-0.1	2	1
0.58	-0.17	2.7	1
0.56	-0.17	3.91	1
0.66	-0.0743	3.21	2
0.59	-0.1	2.49	1
0.57	-0.1	2.98	1
0.59	-0.1	3.39	1
0.73	-0.11	1.48	1
0.57	-0.1	3.47	1
0.65	-0.0921	1.65	1
0.69	-0.17	3.28	1
0.63	-0.17	3.06	1
0.52	-0.13	3.07	1
0.56	-0.17	4.54	2
0.59	0	6.79	1
0.72	-0.12	3.66	1
0.71	0	5.49	1
0.61	-0.17	4.26	1
0.67	-0.12	2.96	1
0.64	-0.1	3.7	1
0.6	-0.17	4.34	1
0.72	-0.12	3.18	2
0.75	-0.11	1.18	1
0.56	-0.17	5.5	1
0.64	-0.17	4.12	1
0.64	-0.17	3.64	1
0.55	-0.1	4.94	1
0.54	-0.0997	4.91	1
0.67	-0.1	3.06	1
0.53	-0.17	5.28	1
0.55	-0.1	5.36	1
0.52	-0.17	7.46	2
0.74	-0.12	2.55	1
0.74	-0.11	1.96	1
0.57	-0.17	3.44	1
0.82	-0.12	3.03	1
0.56	-0.13	3.51	1
0.61	-0.17	4.55	1
0.84	-0.17	3.56	1
0.75	-0.12	2.84	1
0.56	-0.18	4.42	2

0.56	-0.17	2.81	1
0.86	-0.0972	1.57	1
0.57	-0.18	4.68	1
0.58	-0.17	3.94	1
0.58	-0.12	3.43	1
0.57	-0.17	2.81	1
0.58	-0.17	5.48	1
0.54	-0.12	9.09	1
0.57	-0.17	3.46	1
0.66	-0.17	5.43	1
0.66	-0.17	5.43	1
0.58	-0.17	4.12	1
0.65	-0.17	5.64	1
0.58	-0.17	2.7	2
0.57	-0.17	3.42	1
0.57	-0.17	3.46	1
0.7	-0.17	3.92	1
0.78	-0.12	3.18	1
0.73	-0.12	2.84	1

[illegible]

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#CAS	Y (logP(BBB) exp)	Halogenide groups#	HA dependent HDCA-2/SQRT(TMSA) (Zefirov) (all)
57-43-2	0.04	0	0.041
76-74-4	0.12	0	0.042
154-93-8	-0.52	2	0.059
83-67-0	-0.28	0	0.054
50-78-2	-0.50	0	0.046
58-55-9	-0.29	0	0.053
58-08-2	-0.06	0	0.044
69-72-7	-1.10	0	0.042
487-54-7	-0.44	0	0.066
103-90-2	-0.31	0	0.042
15687-27-1	-0.18	0	0.021
76-75-5	-0.14	0	0.037
1622-62-4	0.06	1	0.030
125-33-7	-0.07	0	0.045
51-55-8	-0.06	0	0.034
604-75-1	0.61	1	0.042
28981-97-7	0.04	1	0.027
59-92-7	-0.77	0	0.086
28911-01-5	0.74	2	0.027
29122-68-7	-0.87	0	0.048
1088-11-5	0.50	1	0.027
36507-30-9	-0.35	0	0.045
129618-40-2	0.00	0	0.036
60-80-0	-0.10	0	0.019
18559-94-9	-1.03	0	0.055
22316-55-8	0.36	1	0.027
22316-47-8	0.35	1	0.029
77-10-1	0.68	0	0.003
10457-90-6	1.38	2	0.026
57-47-6	0.08	0	0.028
52-86-8	1.34	2	0.028
525-66-6	0.64	0	0.029
50-33-9	-0.52	0	0.016
68-88-2	0.39	1	0.041
298-46-4	-0.14	0	0.030
56-54-2	-0.46	0	0.036
2095-95-6	1.06	0	0.020
50-47-5	1.20	0	0.011
51481-61-9	-1.42	0	0.050
76-57-3	0.55	0	0.031
50-49-7	1.07	0	0.005
321-64-2	-0.13	0	0.019
69-23-8	1.51	3	0.042
50-48-6	0.89	0	0.003
53-86-1	-1.26	1	0.040
77-07-6	0.00	0	0.023

14759-06-9	0.18	0	0.021
59-05-2	-1.52	0	0.099
117-89-5	1.44	3	0.025
58-15-1	0.00	0	0.020
91-84-9	0.49	0	0.027
50-53-3	1.06	1	0.014
5588-33-0	-0.36	0	0.018
58-40-2	1.23	0	0.011
56-29-1	0.10	0	0.037
57-41-0	-0.04	0	0.027
439-14-5	0.52	1	0.026
57-27-2	-0.16	0	0.047
52-53-9	-0.70	0	0.026
25614-03-3	-1.10	1	0.049

HOMO-1 energy (AM1)	WFOSA Atomic charge (AM1) weighted FOSA	Max net atomic charge (Zefirov) for N atoms	Z to 1
-11.460	56.600	-0.072	1
-11.430	55.990	-0.071	1
-11.010	16.090	0.008	1
-10.710	11.780	-0.070	1
-10.540	17.150	0.000	1
-10.480	12.270	-0.074	1
-10.430	17.660	-0.075	1
-10.430	0.000	0.000	2
-10.250	2.770	-0.091	1
-10.230	17.450	-0.098	1
-10.090	50.790	0.000	1
-9.930	56.290	-0.083	1
-9.860	11.780	0.009	2
-9.820	25.040	-0.094	1
-9.790	36.960	-0.121	1
-9.750	1.660	-0.075	1
-9.720	12.300	-0.055	1
-9.710	4.460	-0.114	1
-9.710	12.070	-0.055	1
-9.700	41.800	-0.102	1
-9.670	5.560	-0.090	1
-9.670	0.351	-0.086	1
-9.640	37.980	-0.086	1
-9.600	22.010	-0.079	2
-9.590	46.150	-0.120	1
-9.590	8.990	-0.089	1
-9.510	13.750	-0.089	1
-9.510	50.690	-0.121	1
-9.480	26.050	-0.121	1
-9.440	39.740	-0.090	1
-9.440	27.270	-0.121	1
-9.430	35.470	-0.120	1
-9.410	34.780	-0.072	1
-9.330	15.870	-0.118	1
-9.310	0.000	-0.088	1
-9.290	30.070	-0.094	1
-9.270	15.570	-0.114	1
-9.260	25.900	-0.114	2
-9.230	36.770	-0.043	1
-9.230	26.260	-0.122	1
-9.180	30.660	-0.114	1
-9.160	24.510	-0.093	1
-9.140	18.340	-0.109	1
-9.130	30.200	-0.125	1
-9.080	17.820	-0.091	1
-9.080	41.290	-0.123	1



-9.080	102.770	-0.110	1
-9.060	20.500	-0.066	1
-9.050	23.440	-0.109	1
-9.010	34.670	-0.077	1
-8.950	24.760	-0.091	1
-8.920	22.890	-0.110	1
-8.880	81.910	-0.110	2
-8.770	23.600	-0.111	1
-10.790	43.180	-0.072	1
-9.860	0.000	-0.072	1
-9.630	11.550	-0.090	2
-9.280	21.450	-0.122	1
-9.200	62.680	-0.061	1
-9.070	88.000	-0.069	1

Kennard-Stone (kX)	Kennard-Stone (Y/kX)	Kennard-Stone (kY/kX)	Duplex
1	1	1	1
1	1	2	1
1	1	1	1
1	1	1	1
1	1	1	1
1	2	2	1
1	1	1	1
1	1	1	1
1	1	1	1
2	2	2	1
1	1	1	1
1	1	1	1
2	1	2	1
1	1	1	1
1	1	1	1
1	1	1	1
1	2	1	1
1	1	1	1
1	1	1	1
1	1	1	1
1	1	1	1
2	2	1	1
1	1	1	1
1	1	1	1
1	1	1	1
1	1	1	1
1	1	1	1
1	1	1	1
1	1	1	1
1	1	1	1
1	1	1	1
1	1	1	1
1	1	1	1
1	1	1	1
1	1	2	1
1	1	1	1
2	1	1	1
1	1	1	1
1	1	1	1
1	1	1	1
2	1	1	1
1	1	1	1
2	2	2	1
1	1	1	1
1	1	1	1



CAS	Y (log(1/EC50) exp)	Relative # of rings	WPSA3 Weighted PPSA (PPSA3*TMSA/1000) (AM1)	Gravitation index (all atom pairs) (AM1)
124-40-3	0.86	0.000	3.126	296.268
120-82-1	2.11	0.083	4.396	1951.630
95-50-1	1.82	0.083	4.755	1544.060
88-06-2	1.75	0.077	4.792	2239.460
87-61-6	2.30	0.083	4.805	2040.510
106-46-7	1.96	0.083	4.862	1457.900
120-83-2	1.07	0.077	4.883	1761.830
62-75-9	1.27	0.000	5.070	711.728
591-35-5	1.85	0.077	5.202	1732.190
108-90-7	0.95	0.083	5.350	1092.340
58-90-2	2.25	0.077	5.440	2868.960
576-24-9	1.51	0.077	5.492	1845.000
75-64-9	0.66	0.000	5.528	614.940
15950-66-0	1.99	0.077	5.761	2357.770
61-82-5	0.32	0.100	5.787	877.953
95-57-8	0.26	0.077	5.829	1369.860
95-77-2	1.71	0.077	5.909	1802.650
109-89-7	0.56	0.000	6.032	594.982
32139-72-3	3.04	0.071	6.207	2624.190
3428-24-8	2.60	0.071	6.310	2091.820
106-48-9	0.53	0.077	6.323	1328.840
3978-67-4	2.85	0.071	6.392	2136.660
2460-49-3	1.80	0.059	6.844	2334.880
87-86-5	2.80	0.077	6.931	3543.500
1198-55-6	3.49	0.071	7.139	3282.510
56961-20-7	2.92	0.071	7.224	2672.880
55-18-5	0.96	0.000	7.306	1070.670
108-91-8	0.70	0.050	7.313	1012.530
108-18-9	0.70	0.000	7.340	981.743
2668-24-8	2.70	0.059	7.361	2932.020
57057-83-7	2.48	0.059	7.497	2952.470
2539-17-5	2.82	0.059	8.387	3578.500
2539-26-6	2.48	0.048	9.968	3612.080
111-92-2	0.83	0.000	11.602	1260.960
260-94-6	2.30	0.130	12.128	2428.970
20679-58-7	3.99	0.000	14.571	3734.680
34014-18-1	3.27	0.032	21.052	3226.700
59-87-0	2.14	0.050	24.597	2657.530
139-91-3	1.44	0.077	33.884	4917.420
15687-40-8	2.96	0.024	58.110	5945.480
87-65-0	0.75	0.077	5.295	1805.330
110-91-8	0.49	0.067	5.518	887.848
108-43-0	0.65	0.077	5.962	1334.210
108-95-2	-0.20	0.077	6.636	978.710
62-53-3	0.69	0.071	7.598	962.448

Polarity parameter (AM1) / square distance Z to 1	(kX)	(Y/kX)	(kY/kX)	Duplex
0.458	1	1	1	1
0.024	1	1	1	1
0.058	1	1	1	2
0.488	1	1	1	1
0.225	1	1	1	1
0.222	1	1	1	1
0.501	2	1	1	1
0.351	1	1	1	1
0.498	2	1	1	1
0.024	1	1	1	1
0.488	1	1	1	1
0.502	1	1	1	1
0.468	1	1	1	1
0.500	1	1	1	1
0.432	1	1	1	1
0.503	1	1	1	1
0.497	1	1	1	1
0.448	1	1	1	2
0.106	1	1	1	1
0.099	1	1	1	1
0.499	1	1	1	1
0.035	1	1	1	1
0.512	1	1	1	1
0.487	1	1	1	1
0.106	1	1	1	1
0.104	1	1	1	2
0.346	1	1	1	1
0.472	1	1	1	1
0.444	1	1	1	1
0.498	1	1	1	1
0.506	1	1	1	1
0.496	1	1	1	1
0.500	2	1	1	1
0.454	1	1	1	1
0.040	1	1	1	1
0.418	1	1	1	2
0.033	1	1	1	1
0.019	1	1	1	1
0.662	1	1	1	2
0.092	2	1	1	1
0.490	1	2	2	1
0.409	1	2	2	1
0.500	1	2	2	1
0.502	1	2	2	1
0.514	2	2	2	1

Model #	Ref	Splitting Algorithm	Model's equation	n <sub>training</sub>
Model 1	b,c,f	Z:1 (Y)	y=Log(LC50) a=Average Bond Order b=Highest Total Interaction c=LPSA (Low Polarity Part of SASA) d=Count of H-Acceptor Sites e=logP	n <sub>training</sub> 423
		Kennard-Stone (kX)	y=0.963-3.478a-0.319b-0.002c-0.157d-0.637e	423
		Kennard-Stone (Y/kX)	y=0.940-3.275a-0.307b-0.003c-0.169d-0.624e	423
		Kennard-Stone (kY/kX)	y=0.849-3.226a-0.308b-0.002c-0.171d-0.623e	423
		Duplex (kX)	y=0.883-3.195a-0.304b-0.003c-0.167d-0.625e	423
		Duplex (kX)	y=0.764-3.260a-0.316b-0.002c-0.146d-0.640e	423
Model 2	a	Z:1 (Y)	y=LogK <sub>OW</sub> a=Dipole moment b=Solvent Accessible Surface	n <sub>training</sub> 178
		Kennard-Stone (kX)	y=-0.359-0.122a+0.025b	178
		Kennard-Stone (Y/kX)	y=-0.238-0.115a+0.024b	178
		Kennard-Stone (kY/kX)	y=-0.270-0.123a+0.024b	178
		Duplex (kX)	y=-0.288-0.125a+0.025b	178
		Duplex (kX)	y=-0.295-0.129a+0.025b	178
Model 3	a	Z:1 (Y)	y=LogK <sub>OA</sub> a=Energy of HOMO b=Mean Polarizability	n <sub>training</sub> 77
		Kennard-Stone (kX)	y=7.311+0.741a+0.286b	77
		Kennard-Stone (Y/kX)	y=7.005+0.719a+0.288b	77
		Kennard-Stone (kY/kX)	y=7.005+0.719a+0.288b	77
		Duplex (kX)	y=7.400+0.762a+0.289b	77
		Duplex (kX)	y=9.308+0.948a+0.285b	77
Model 4	b,c,g	Z:1 (Y)	y=LogER-RBA a=Average Information Content (order 1) b=Number of Rings c=Relative ALFA Polarizability (DIP) (AM1) d=Max Net Atomic Charge (Zefirov) for O Atoms e=logP	n <sub>training</sub> 62
		Kennard-Stone (kX)	y=-19.003+2.106a+0.782b+7.276c-13.685d+0.842e	62
		Kennard-Stone (Y/kX)	y=-19.427+2.112a+0.711b+7.901c-14.486d+0.842e	62
		Kennard-Stone (kY/kX)	y=-19.466+2.186a+0.754b+7.641c-14.383d+0.832e	62
		Duplex (kX)	y=-19.539+2.127a+0.754b+7.962c-14.661d+0.835e	62
		Duplex (kX)	y=-18.912+2.032a+0.775b+7.054c-14.634d+0.857e	62
Model 5	b,c,d	Z:1 (Y)	y=LogBB a=# Halogenide Groups b=HA Dependent HDCA-2/SQRT(TMSA) (Zefirov) (all) c=Energy of (HOMO-1) d=WFOSA (Weighted FOSA) Atomic Charge (AM1) e=Max Net Atomic Charge (Zefirov) for N Atoms	n <sub>training</sub> 54
		Kennard-Stone (kX)	y=-3.018+0.399a-25.709b-0.324c-0.006d-9.969e	54
		Kennard-Stone (Y/kX)	y=-3.278+0.396a-25.230b-0.342c-0.007d-10.848e	54
		Kennard-Stone (kY/kX)	y=-3.062+0.395a-26.487b-0.337c-0.008d-10.039e	54
		Duplex (kX)	y=-3.069+0.390a-25.791b-0.324c-0.007d-10.904e	54
		Duplex (kX)	y=-2.584+0.413a-25.610b-0.282c-0.006d-9.403e	54

Model 6

		y=Log(1/EC50)	
		a=Relative # Rings	
		b=WPSA3	
		c=Gravitation Index	
		d=Polarity Parameter	n <sub>training</sub>
b,c,e	Z:1 (Y)	y=1.657-9.959a-0.085b+0.001c-2.543d	40
	Kennard-Stone (kX)	y=1.624-8.311a-0.077b+0.001c-2.400d	40
	Kennard-Stone (Y/kX)	y=1.624-8.311a-0.077b+0.001c-2.400d	40
	Kennard-Stone (kY/kX)	y=1.624-8.311a-0.077b+0.001c-2.400d	40
	Duplex (kX)	y=1.508-6.787a-0.070b+0.001c-2.333d	40

$n_{\text{test}}$	$k_{\text{descriptors}}$	$R^2$	$Q^2_{\text{CV}}$	$Q^2_{\text{EXT}}$	$\text{RMSE}_{\text{C}}$	$\text{RMSE}_{\text{CV}}$	$\text{RMSE}_{\text{P}}$	$s$	$\text{TSS}_{\text{EXT}}$	$\text{PRESS}_{\text{EXT}}$
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$n_{\text{test}}$	$k_{\text{descriptors}}$	$R^2$	$Q^2_{\text{CV}}$	$Q^2_{\text{EXT}}$	$\text{RMSE}_{\text{C}}$	$\text{RMSE}_{\text{CV}}$	$\text{RMSE}_{\text{P}}$	$s$	$\text{TSS}_{\text{EXT}}$	$\text{PRESS}_{\text{EXT}}$
46	5	0.763	0.754	0.699	0.680	0.693	0.696	0.685	74.088	22.278
46	5	0.760	0.751	0.696	0.692	0.705	0.579	0.697	50.561	15.398
46	5	0.755	0.744	0.776	0.699	0.713	0.498	0.704	50.826	11.386
46	5	0.757	0.747	0.767	0.699	0.713	0.486	0.704	46.619	10.877
46	5	0.753	0.740	0.728	0.655	0.672	0.894	0.660	134.941	36.747

$n_{\text{test}}$	$k_{\text{descriptors}}$	$R^2$	$Q^2_{\text{CV}}$	$Q^2_{\text{EXT}}$	$\text{RMSE}_{\text{C}}$	$\text{RMSE}_{\text{CV}}$	$\text{RMSE}_{\text{P}}$	$s$	$\text{TSS}_{\text{EXT}}$	$\text{PRESS}_{\text{EXT}}$
59	2	0.920	0.918	0.925	0.315	0.321	0.303	0.318	71.469	5.399
59	2	0.920	0.917	0.926	0.316	0.322	0.296	0.319	69.751	5.176
59	2	0.925	0.922	0.884	0.332	0.337	0.239	0.335	28.936	3.356
59	2	0.924	0.921	0.894	0.335	0.341	0.224	0.338	28.046	2.969
59	2	0.928	0.926	0.900	0.300	0.305	0.344	0.303	69.649	6.964

$n_{\text{test}}$	$k_{\text{descriptors}}$	$R^2$	$Q^2_{\text{CV}}$	$Q^2_{\text{EXT}}$	$\text{RMSE}_{\text{C}}$	$\text{RMSE}_{\text{CV}}$	$\text{RMSE}_{\text{P}}$	$s$	$\text{TSS}_{\text{EXT}}$	$\text{PRESS}_{\text{EXT}}$
26	2	0.972	0.970	0.961	0.320	0.333	0.376	0.326	93.379	3.675
26	2	0.976	0.974	0.881	0.330	0.343	0.369	0.337	29.587	3.536
26	2	0.973	0.971	0.930	0.346	0.359	0.303	0.353	34.321	2.393
26	2	0.971	0.969	0.954	0.347	0.360	0.303	0.354	51.297	2.379
26	2	0.964	0.961	0.979	0.341	0.356	0.322	0.348	127.284	2.687

$n_{\text{test}}$	$k_{\text{descriptors}}$	$R^2$	$Q^2_{\text{CV}}$	$Q^2_{\text{EXT}}$	$\text{RMSE}_{\text{C}}$	$\text{RMSE}_{\text{CV}}$	$\text{RMSE}_{\text{P}}$	$s$	$\text{TSS}_{\text{EXT}}$	$\text{PRESS}_{\text{EXT}}$
6	5	0.797	0.726	0.422	0.808	0.939	0.846	0.850	7.422	4.290
6	5	0.789	0.723	0.738	0.803	0.919	0.914	0.844	19.139	5.016
6	5	0.781	0.714	0.544	0.833	0.952	0.518	0.877	3.530	1.609
6	5	0.785	0.721	0.333	0.828	0.944	0.604	0.872	3.277	2.186
6	5	0.779	0.701	0.805	0.808	0.940	0.865	0.850	23.080	4.493

$n_{\text{test}}$	$k_{\text{descriptors}}$	$R^2$	$Q^2_{\text{CV}}$	$Q^2_{\text{EXT}}$	$\text{RMSE}_{\text{C}}$	$\text{RMSE}_{\text{CV}}$	$\text{RMSE}_{\text{P}}$	$s$	$\text{TSS}_{\text{EXT}}$	$\text{PRESS}_{\text{EXT}}$
6	5	0.752	0.679	0.721	0.360	0.410	0.377	0.382	3.056	0.852
6	5	0.757	0.685	0.640	0.361	0.411	0.360	0.383	2.163	0.779
6	5	0.752	0.679	0.619	0.373	0.424	0.264	0.395	1.097	0.418
6	5	0.757	0.684	0.468	0.370	0.422	0.297	0.393	0.992	0.527
6	5	0.739	0.664	0.812	0.375	0.426	0.230	0.398	1.690	0.318



$n_{\text{test}}$	$k_{\text{descriptors}}$	$R^2$	$Q^2_{\text{CV}}$	$Q^2_{\text{EXT}}$	$\text{RMSE}_{\text{C}}$	$\text{RMSE}_{\text{CV}}$	$\text{RMSE}_{\text{P}}$	$s$	$\text{TSS}_{\text{EXT}}$	$\text{PRESS}_{\text{EXT}}$
5	4	0.924	0.881	0.629	0.282	0.352	0.515	0.301	3.575	1.327
5	4	0.900	0.864	-0.114	0.300	0.350	0.368	0.321	0.608	0.678
5	4	0.900	0.864	-0.114	0.300	0.350	0.368	0.321	0.608	0.678
5	4	0.900	0.864	-0.114	0.300	0.350	0.368	0.321	0.608	0.678
5	4	0.903	0.874	0.873	0.300	0.342	0.425	0.321	7.120	0.902

GOODNESS OF FIT STATISTICS:

$$RMSEC = \sqrt{\frac{\sum_{i=1}^n (y_i^{obs} - y_i^{pred})^2}{n}}$$

$$R^2 = 1 - \frac{\sum_{i=1}^n (y_i^{obs} - y_i^{pred})^2}{\sum_{i=1}^n (y_i^{obs} - y_{obs}^{mean})^2}$$

ROBUSTNESS STATISTICS:

$$RMSECV = \sqrt{\frac{\sum_{i=1}^n (y_i^{obs} - y_i^{cv})^2}{n}}$$

$$Q_{CV}^2 = \sqrt{\frac{\sum_{i=1}^n (y_i^{obs} - y_i^{ppred-cv})^2}{\sum_{i=1}^n (y_i^{obs} - y_{obs}^{mean})^2}}$$

PREDICTIVITY STATISTICS:

$$RMSEP = \sqrt{\frac{\sum_{i=1}^{n_v} (y_i^{obs} - y_i^{pred})^2}{n_v}}$$

$$Q_{EXT}^2 = 1 - \frac{\sum_{i=1}^{n_v} (y_i^{obs} - y_i^{pred})^2}{\sum_{i=1}^{n_v} (y_i^{obs} - y_{obs}^{mean})^2}$$

$$(y_i^{obs} - y_i^{pred})^2$$

$$(y_i^{obs} - y_{obs}^{mean})^2$$

$$(y_i^{obs} - y_i^{ppred - cv})^2$$

$$(y_i^{obs} - y_{obs}^{mean})^2$$

$$\sum_{i=1}^{n_v} (y_i^{obs} - y_i^{pred})^2$$

$$\sum_{i=1}^{n_v} (y_i^{obs} - y_{obs}^{mean})^2$$